

Bulk-boundary correspondence of topologically trivial insulators

Haruki Watanabe
University of Tokyo

[HW](#) and S. Ono, Phys. Rev. B 102, 165120 (2020)
[HW](#) and H. C. Po, arXiv:2009.04845



Seishiro Ono

The University of Tokyo



Hoi Chun Po

The Hong Kong University
of Science and Technology

Variety of condensed matter

PERIODIC TABLE OF ELEMENTS

PubChem

1 H Hydrogen Nonmetal																	2 He Helium Noble Gas	
3 Li Lithium Alkali Metal	4 Be Beryllium Alkaline Earth Metal																	10 Ne Neon Noble Gas
11 Na Sodium Alkali Metal	12 Mg Magnesium Alkaline Earth Metal																	18 Ar Argon Noble Gas
19 K Potassium Alkali Metal	20 Ca Calcium Alkaline Earth Metal	21 Sc Scandium Transition Metal	22 Ti Titanium Transition Metal	23 V Vanadium Transition Metal	24 Cr Chromium Transition Metal	25 Mn Manganese Transition Metal	26 Fe Iron Transition Metal	27 Co Cobalt Transition Metal	28 Ni Nickel Transition Metal	29 Cu Copper Transition Metal	30 Zn Zinc Transition Metal	31 Ga Gallium Post-Transition Metal	32 Ge Germanium Metalloid	33 As Arsenic Metalloid	34 Se Selenium Nonmetal	35 Br Bromine Halogen	36 Kr Krypton Noble Gas	
37 Rb Rubidium Alkali Metal	38 Sr Strontium Alkaline Earth Metal	39 Y Yttrium Transition Metal	40 Zr Zirconium Transition Metal	41 Nb Niobium Transition Metal	42 Mo Molybdenum Transition Metal	43 Tc Technetium Transition Metal	44 Ru Ruthenium Transition Metal	45 Rh Rhodium Transition Metal	46 Pd Palladium Transition Metal	47 Ag Silver Transition Metal	48 Cd Cadmium Transition Metal	49 In Indium Post-Transition Metal	50 Sn Tin Post-Transition Metal	51 Sb Antimony Metalloid	52 Te Tellurium Metalloid	53 I Iodine Halogen	54 Xe Xenon Noble Gas	
55 Cs Cesium Alkali Metal	56 Ba Barium Alkaline Earth Metal		72 Hf Hafnium Transition Metal	73 Ta Tantalum Transition Metal	74 W Tungsten Transition Metal	75 Re Rhenium Transition Metal	76 Os Osmium Transition Metal	77 Ir Iridium Transition Metal	78 Pt Platinum Transition Metal	79 Au Gold Transition Metal	80 Hg Mercury Transition Metal	81 Tl Thallium Post-Transition Metal	82 Pb Lead Post-Transition Metal	83 Bi Bismuth Metalloid	84 Po Polonium Metalloid	85 At Astatine Halogen	86 Rn Radon Noble Gas	
87 Fr Francium Alkali Metal	88 Ra Radium Alkaline Earth Metal		104 Rf Rutherfordium Transition Metal	105 Db Dubnium Transition Metal	106 Sg Seaborgium Transition Metal	107 Bh Bohrium Transition Metal	108 Hs Hassium Transition Metal	109 Mt Meitnerium Transition Metal	110 Ds Darmstadtium Transition Metal	111 Rg Roentgenium Transition Metal	112 Cn Copernicium Transition Metal	113 Nh Nihonium Post-Transition Metal	114 Fl Flerovium Post-Transition Metal	115 Mc Moscovium Post-Transition Metal	116 Lv Livermorium Post-Transition Metal	117 Ts Tennessine Halogen	118 Og Oganesson Noble Gas	
		57 La Lanthanum Lanthanide	58 Ce Cerium Lanthanide	59 Pr Praseodymium Lanthanide	60 Nd Neodymium Lanthanide	61 Pm Promethium Lanthanide	62 Sm Samarium Lanthanide	63 Eu Europium Lanthanide	64 Gd Gadolinium Lanthanide	65 Tb Terbium Lanthanide	66 Dy Dysprosium Lanthanide	67 Ho Holmium Lanthanide	68 Er Erbium Lanthanide	69 Tm Thulium Lanthanide	70 Yb Ytterbium Lanthanide	71 Lu Lutetium Lanthanide		
		89 Ac Actinium Actinide	90 Th Thorium Actinide	91 Pa Protactinium Actinide	92 U Uranium Actinide	93 Np Neptunium Actinide	94 Pu Plutonium Actinide	95 Am Americium Actinide	96 Cm Curium Actinide	97 Bk Berkelium Actinide	98 Cf Californium Actinide	99 Es Einsteinium Actinide	100 Fm Fermium Actinide	101 Md Mendelevium Actinide	102 No Nobelium Actinide	103 Lr Lawrencium Actinide		

1
H
Hydrogen
Nonmetal

Atomic Number
Symbol
Name
Chemical Group Block

230 The Space Group List Project

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by Frank Hoffmann

Diagram illustrating the variety of condensed matter structures, showing 230 space groups. Each entry includes a space group symbol (e.g., P1, P2, P3, P4, C2, Pm, Pc, Cm, Cc, P2/m, P2/m, C2/m, P2/c, P2/c) and a corresponding 3D lattice structure visualization.

“Quantum Mechanical Systems”
at “Large Quantum Number”

Variety of condensed matter

PERIODIC TABLE OF ELEMENTS

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H Symbol
Hydrogen Name
Nonmetal Chemical Group Block

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38 Sr Strontium Alkaline Earth Metal

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88 Ra Radium Alkaline Earth Metal

71 Lu Lutetium Lanthanide
72 Hf Hafnium Transition Metal

89 Ac Actinium Actinide
90 Th Thorium Actinide

230 The Space Group List Project

by Frank Hoffmann

Space group symbols and numbers: P1 (#1), P1 (#2), P2 (#3), P2 (#4), C2 (#5), Pm (#6), Pc (#7), Cm (#8), Cc (#9), P2/m (#10), P2/m (#11), C2/m (#12), P2/c (#13), P2/c (#14), P222 (#16), P222 (#17), P2,2,2 (#18), P2,2,2 (#19), C222 (#20), C222 (#21), F222 (#22), F222 (#23), I2,2,2 (#24), Pmm2 (#25), Pmc2 (#26), Pcc2 (#27), Pma2 (#28), P422 (#29), P422 (#30), P422 (#31), P422 (#32), P422 (#33), P422 (#34), Cmm2 (#35), Cmc2 (#36), Ccc2 (#37), Amm2 (#38), Abm2 (#39), Ama2 (#40), Aca2 (#41), Fmm2 (#42), P422 (#43), P422 (#44), P422 (#45), P422 (#46), P422 (#47), P422 (#48), P422 (#49), P422 (#50), P422 (#51), P422 (#52), P422 (#53), P422 (#54), P422 (#55), P422 (#56), P422 (#57), P422 (#58), P422 (#59), P422 (#60), P422 (#61), P422 (#62), P422 (#63), P422 (#64), P422 (#65), P422 (#66), P422 (#67), P422 (#68), P422 (#69), P422 (#70), P422 (#71), P422 (#72), P422 (#73), P422 (#74), P422 (#75), P422 (#76), P422 (#77), P422 (#78), P422 (#79), P422 (#80), P422 (#81), P422 (#82), P422 (#83), P422 (#84), P422 (#85), P422 (#86), P422 (#87), P422 (#88), P422 (#89), P422 (#90), P422 (#91), P422 (#92), P422 (#93), P422 (#94), P422 (#95), P422 (#96), P422 (#97), P422 (#98), P422 (#99), P422 (#100), P422 (#101), P422 (#102), P422 (#103), P422 (#104), P422 (#105), P422 (#106), P422 (#107), P422 (#108), P422 (#109), P422 (#110), P422 (#111), P422 (#112), P422 (#113), P422 (#114), P422 (#115), P422 (#116), P422 (#117), P422 (#118), P422 (#119), P422 (#120), P422 (#121), P422 (#122), P422 (#123), P422 (#124), P422 (#125), P422 (#126), P422 (#127), P422 (#128), P422 (#129), P422 (#130), P422 (#131), P422 (#132), P422 (#133), P422 (#134), P422 (#135), P422 (#136), P422 (#137), P422 (#138), P422 (#139), P422 (#140), P422 (#141), P422 (#142), P422 (#143), P422 (#144), P422 (#145), P422 (#146), P422 (#147), P422 (#148), P422 (#149), P422 (#150), P422 (#151), P422 (#152), P422 (#153), P422 (#154), P422 (#155), P422 (#156), P422 (#157), P422 (#158), P422 (#159), P422 (#160), P422 (#161), P422 (#162), P422 (#163), P422 (#164), P422 (#165), P422 (#166), P422 (#167), P422 (#168), P422 (#169), P422 (#170), P422 (#171), P422 (#172), P422 (#173), P422 (#174), P422 (#175), P422 (#176), P422 (#177), P422 (#178), P422 (#179), P422 (#180), P422 (#181), P422 (#182), P422 (#183), P422 (#184), P422 (#185), P422 (#186), P422 (#187), P422 (#188), P422 (#189), P422 (#190), P422 (#191), P422 (#192), P422 (#193), P422 (#194), P422 (#195), P422 (#196), P422 (#197), P422 (#198), P422 (#199), P422 (#200), P422 (#201), P422 (#202), P422 (#203), P422 (#204), P422 (#205), P422 (#206), P422 (#207), P422 (#208), P422 (#209), P422 (#210), P422 (#211), P422 (#212), P422 (#213), P422 (#214), P422 (#215), P422 (#216), P422 (#217), P422 (#218), P422 (#219), P422 (#220), P422 (#221), P422 (#222), P422 (#223), P422 (#224), P422 (#225), P422 (#226), P422 (#227), P422 (#228), P422 (#229), P422 (#230).

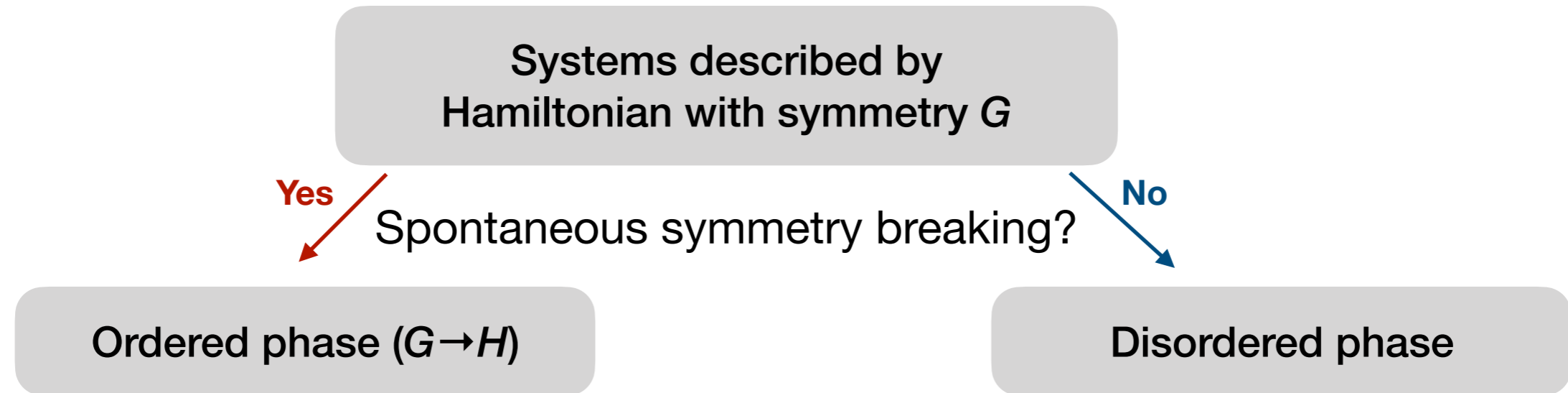
“Quantum Mechanical Systems”
at “Large Quantum Number”

(The topic today is unfortunately

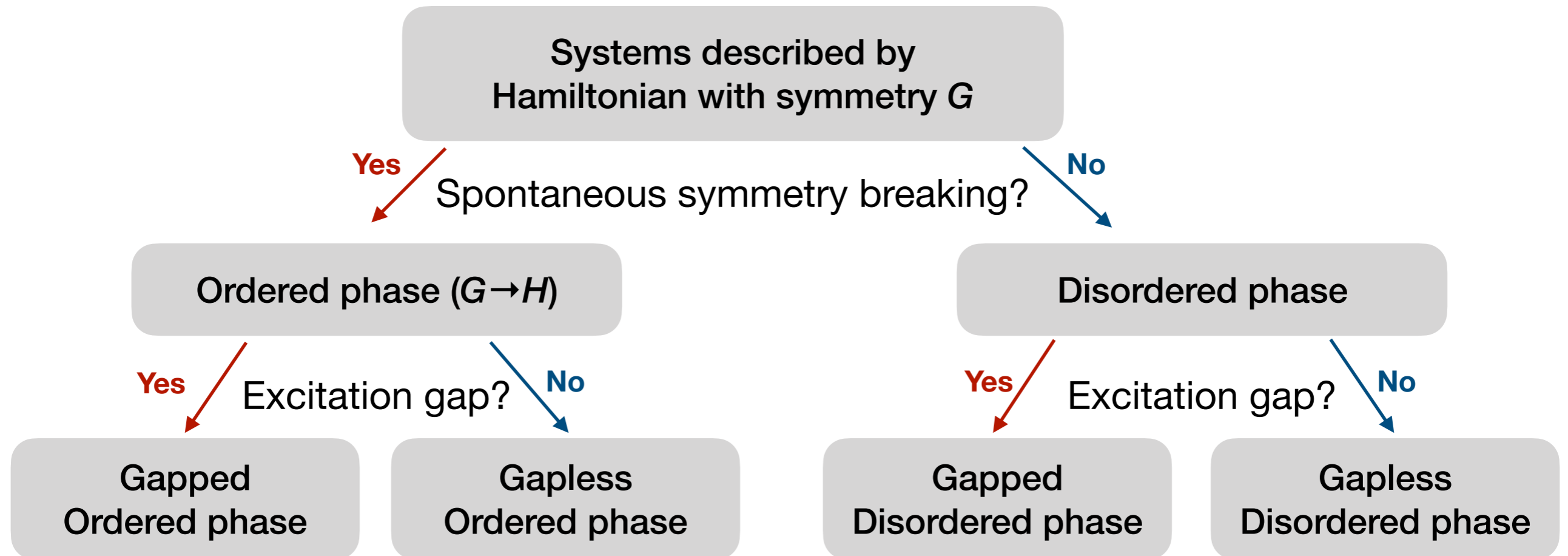
not really quantum or with large quantum number)

More information at
crystalsymmetry.wordpress.com

Classification of $T=0$ phases



Classification of $T=0$ phases



Classification of $T=0$ phases

Systems described by
Hamiltonian with symmetry G

Yes
Spontaneous symmetry breaking?

No

Ordered phase ($G \rightarrow H$)

Disordered phase

Yes
Excitation gap?

No

Yes
Excitation gap?

No

Gapped
Ordered phase

Gapless
Ordered phase

Gapped
Disordered phase

Gapless
Disordered phase

- Continuous symmetry breaking
- ...

- Fermi liquids
- Critical phases
- Gapless spin liquids
- ...

Yes
Degeneracy
more than $|G/H|$?

No

Yes
Degeneracy?

No

Long-range entangled
phases

Short-range entangled
phases

Topologically ordered phases (FQHE, QSL, ...)
Fracton topological orders

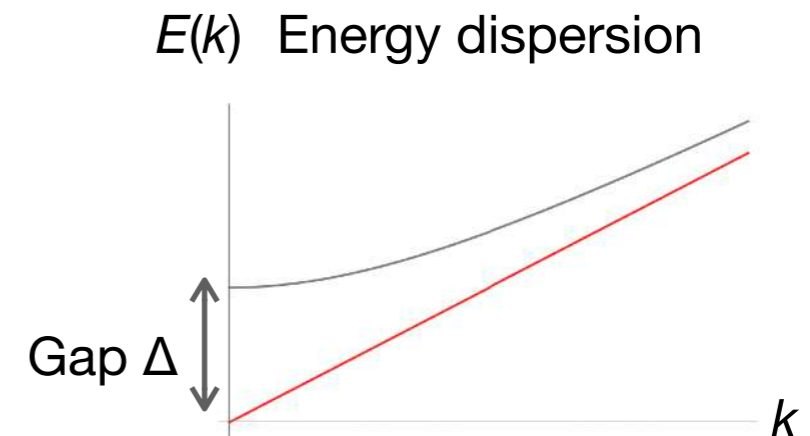
- Trivial phases
- Topological insulators
- Symmetry-protected topological phases

Nambu-Goldstone modes in relativistic systems

Upon spontaneous breaking of G into H

Counting rule: $n_{\text{NGM}} = n_{\text{BG}}$

$$n_{\text{BG}} \equiv \dim G/H = \dim G - \dim H$$



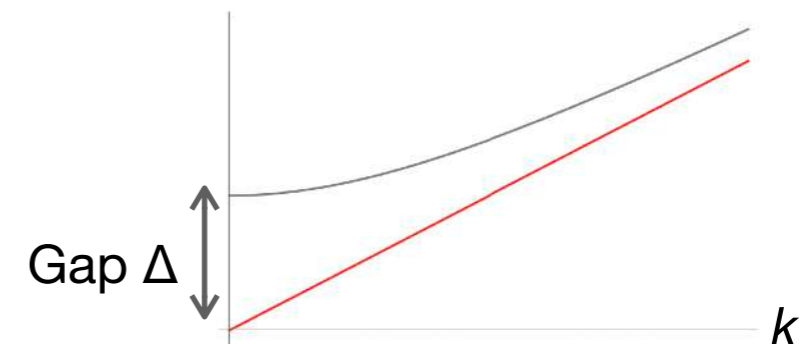
Nambu-Goldstone modes in relativistic systems

Upon spontaneous breaking of G into H

Counting rule: $n_{\text{NGM}} = n_{\text{BG}}$

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$E(k)$ Energy dispersion



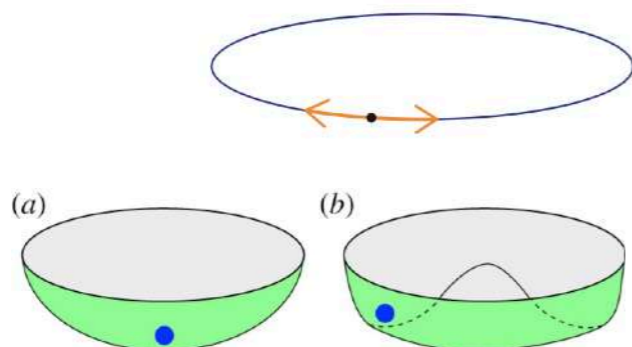
low-E effective Lagrangian

$$\mathcal{L}_{\text{eff}} = \sum_{a,b} \sum_{\mu,\nu} \frac{1}{2} g_{ab} \eta^{\mu\nu} \omega_{\mu}^a \omega_{\nu}^b + \dots,$$

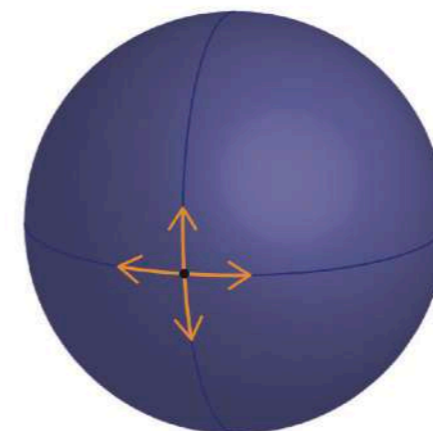
Maurer–Cartan one-form

$$\sum_i \omega_{\mu}^i T_i \equiv -iU^{\dagger} \partial_{\mu} U, \quad U(\pi) \equiv e^{i \sum_a \pi^a T_a}.$$

a $G/H = S^1$



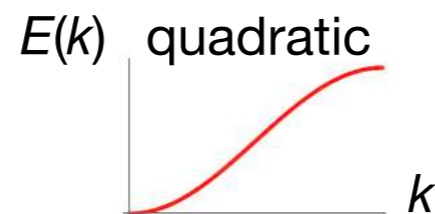
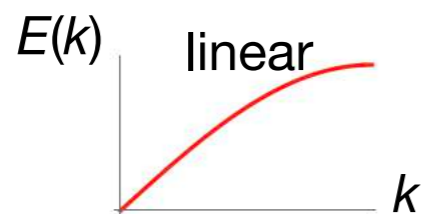
c $G/H = S^2$



Nambu-Goldstone modes in *non-relativistic* systems

HW, H. Murayama, PRL (2012), HW, Annual Review of Condensed Matter Physics (2020)

$$n_{\text{NGM}} = n_{\text{BG}} - \frac{1}{2} \text{rank} \rho \quad \rho_{ij} \equiv -i \frac{1}{V} \langle [\hat{Q}_i, \hat{Q}_j] \rangle = \sum_k f_{ij}^k \frac{\langle \hat{Q}_k \rangle}{V}$$



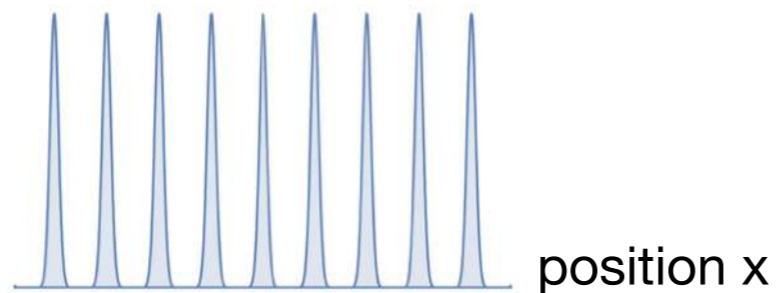
$$\rho = \left(\begin{array}{cc|cc|cc} 0 & \lambda_1 & & & & \\ -\lambda_1 & 0 & & & & \\ & & 0 & \lambda_2 & & \\ & & -\lambda_2 & 0 & & \\ & & & & \ddots & \\ & & & & & 0 & \lambda_m \\ & & & & & -\lambda_m & 0 \\ \hline & & & & & & 0 \end{array} \right)$$

Quantum Time Crystals

F. Wilczek. PRL (2012)

(conventional) crystal

$\langle \rho(x) \rangle$: ground-state expectation
value of density of ions, atoms, ...

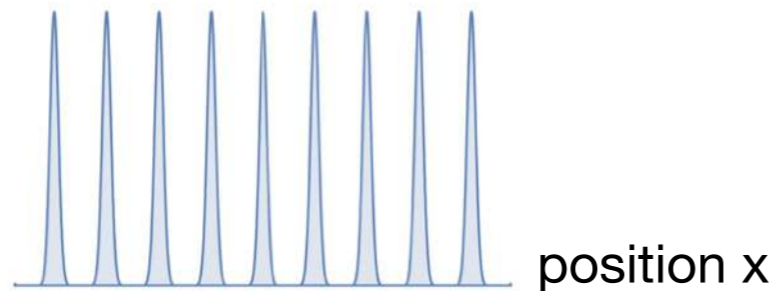


Quantum Time Crystals

F. Wilczek, PRL (2012)

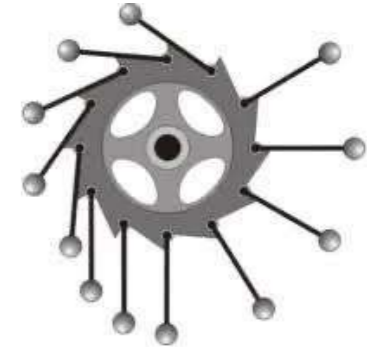
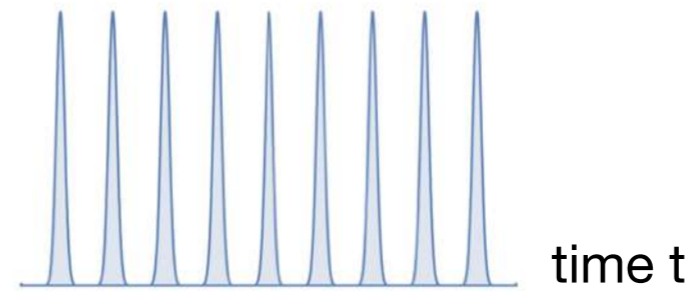
(conventional) crystal

$\langle \rho(x) \rangle$: ground-state expectation value of density of ions, atoms, ...



Quantum Time Crystal

$\langle O(t) \rangle$: ground-state expectation value of an observable

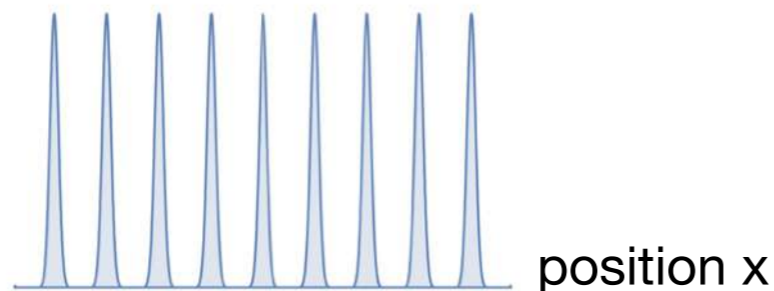


Quantum Time Crystals

F. Wilczek, PRL (2012)

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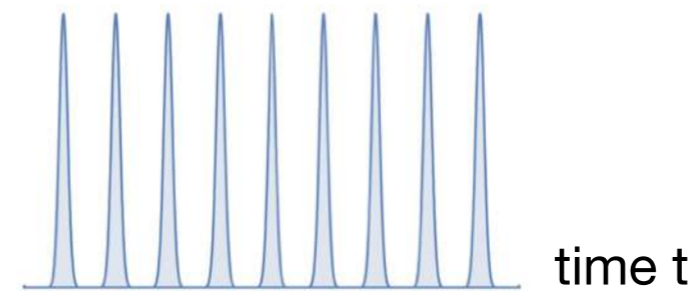
$\langle \rho(x) \rangle$: ground-state expectation value of density of ions, atoms, ...



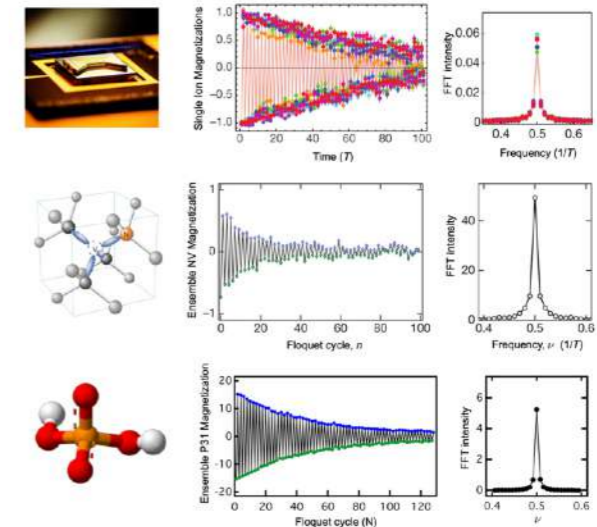
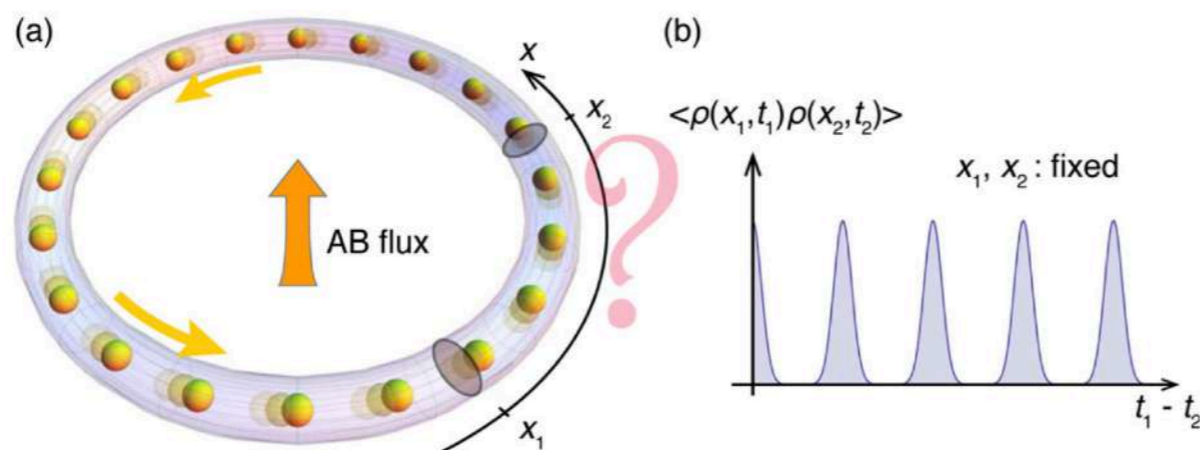
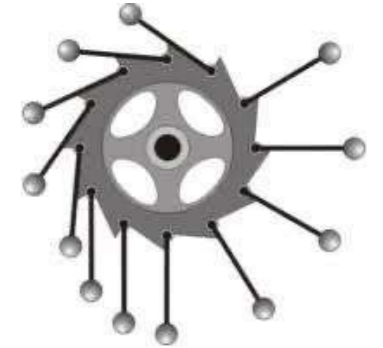
$$\lim_{V \rightarrow \infty} \langle \hat{\phi}(\vec{x}, 0) \hat{\phi}(\vec{x}', 0) \rangle \rightarrow f(\vec{x} - \vec{x}')$$

Quantum Time Crystal

$\langle O(t) \rangle$: ground-state expectation value of an observable



$$\lim_{V \rightarrow \infty} \langle \hat{\phi}(\vec{x}, t) \hat{\phi}(0, 0) \rangle \rightarrow f(t)$$



We showed $f(t)$ is time-independent \rightarrow absence of QTC

HW, M. Oshikawa, PRL (2015)

\rightarrow Recent realization of Discrete Time Crystals (in driven systems)

D. V. Else, et al, ARCMP (2020)

Classification of $T=0$ phases

Systems described by
Hamiltonian with symmetry G

Yes
Spontaneous symmetry breaking?

No

Ordered phase ($G \rightarrow H$)

Disordered phase

Yes
Excitation gap?

No

Yes
Excitation gap?

No

Gapped
Ordered phase

Gapless
Ordered phase

Gapped
Disordered phase

Gapless
Disordered phase

- Continuous symmetry breaking
- ...

- Fermi liquids
- Critical phases
- Gapless spin liquids
- ...

Yes
Degeneracy
more than $|G/H|$?

No

Yes
Degeneracy?

No

Long-range entangled
phases

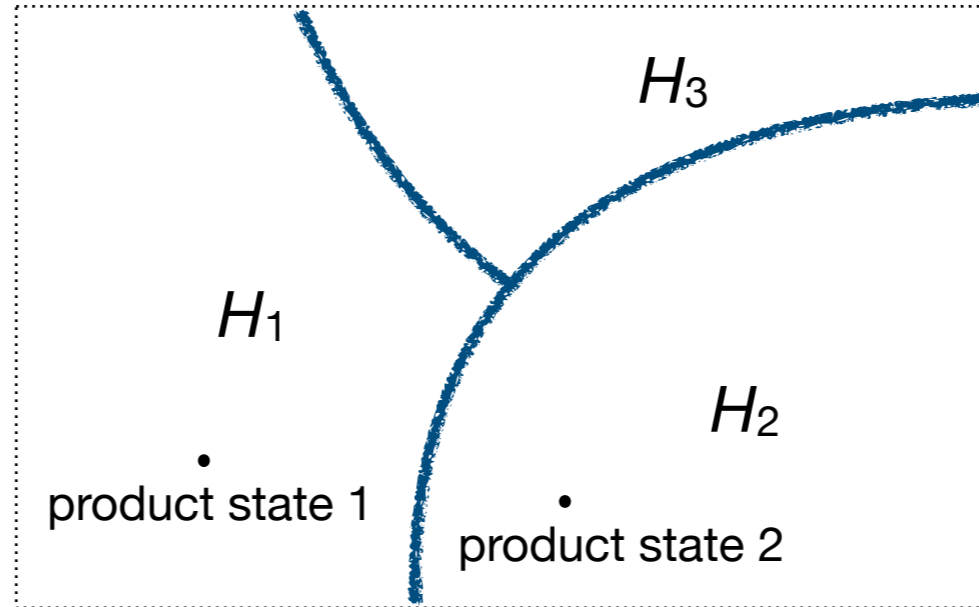
Short-range entangled
phases

Topologically ordered phases (FQHE, QSL, ...)
Fracton topological orders

- Trivial phases
- Topological insulators
- Symmetry-protected topological phases

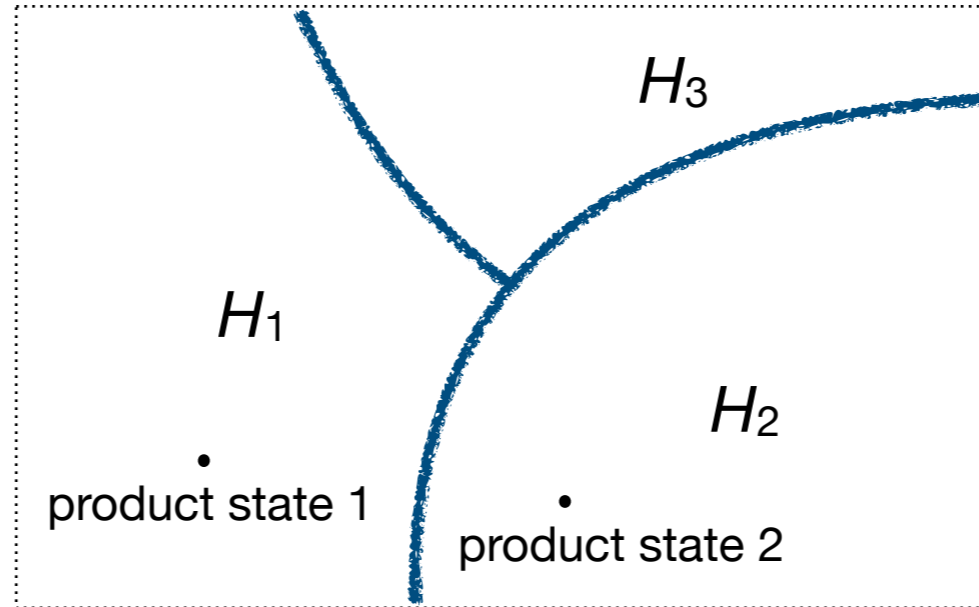
Classification of short-range entangled phases

- Assume a symmetry G and excitation gap Δ
- $H_1 \sim H_2$ if H_1 and H_2 are connected without breaking symmetry G or closing gap Δ (with or without ancillas)

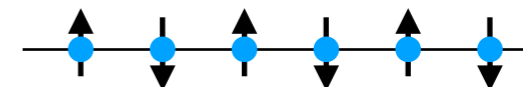


Classification of short-range entangled phases

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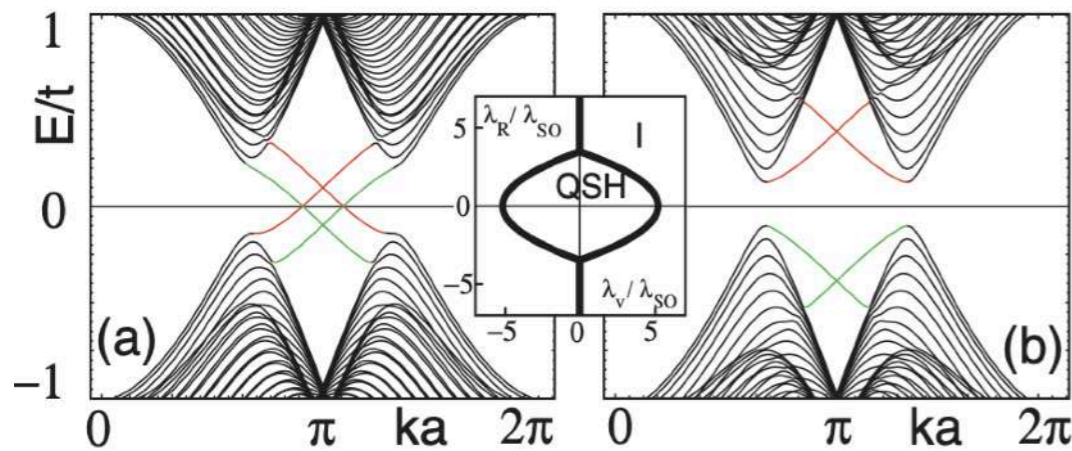
- *Trivial phases* are connected to a real-space **product state**.



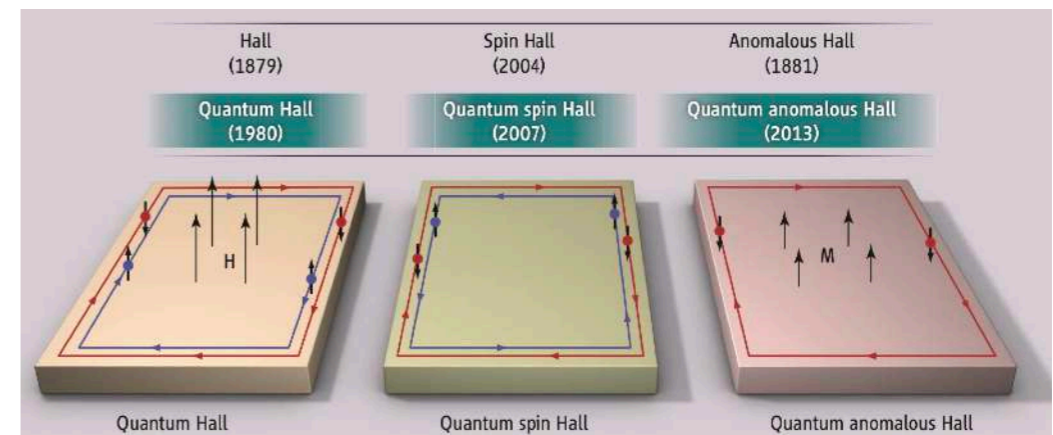
- *Topological phases* contain irremovable **quantum entanglement**.

Bulk-boundary correspondence of topological phases

- 2D topological insulator

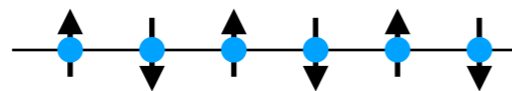


C. L. Kane and E. J. Mele, PRL (2005)



S. Oh, Science (2013)

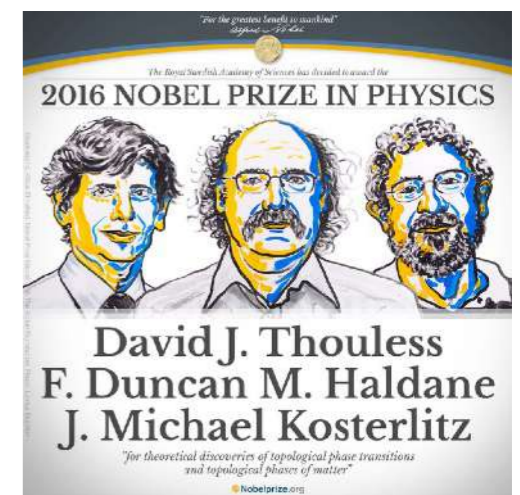
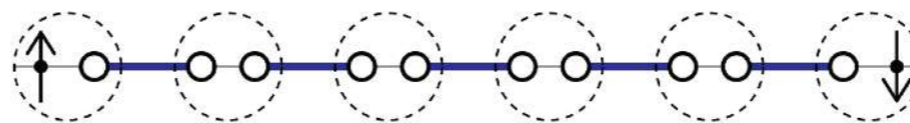
- Haldane phase



$S = 1$ Heisenberg model

$S = 1/2$ edge spin

$$\hat{H} = J \sum_n \hat{\mathbf{s}}_n \cdot \hat{\mathbf{s}}_{n+1}$$

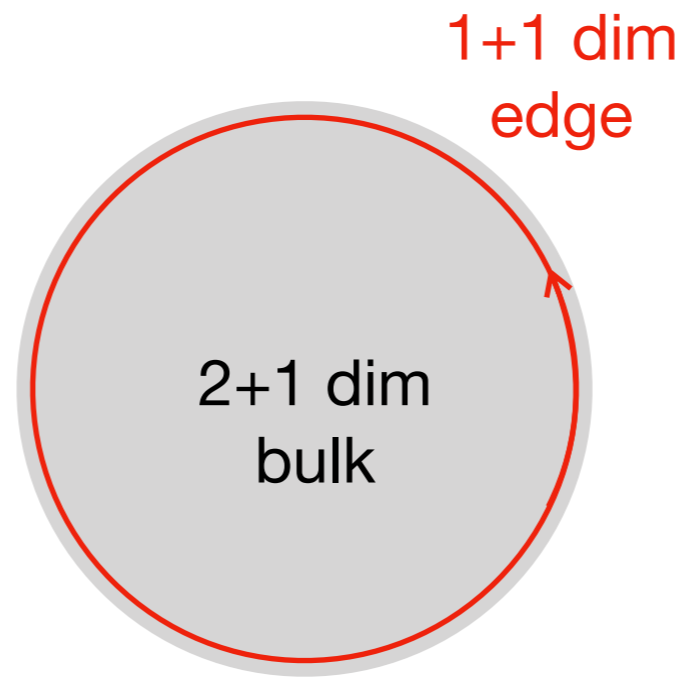


Bulk topology implies nontrivial boundary.

Boundary states(=degrees of freedom) / surface topological order

Bulk-boundary correspondence

— anomaly inflow —



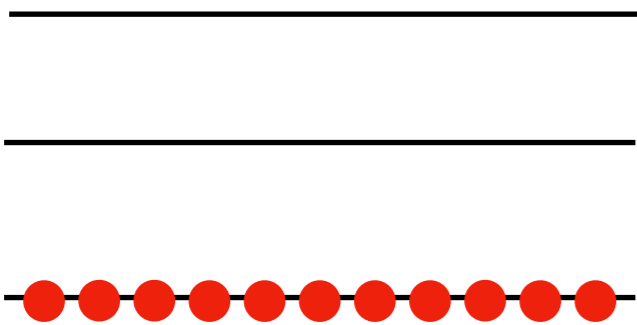
Bulk-boundary correspondence

— anomaly inflow —

**2+1 dim bulk:
Chern Simons theory**

$$I_{\text{eff}} = \frac{k}{4\pi} \int_{M_3} d^3x \epsilon^{ijk} A_i \partial_j A_k.$$

⋮



- Gauge invariant if no boundary
- Gauge dependent with boundary

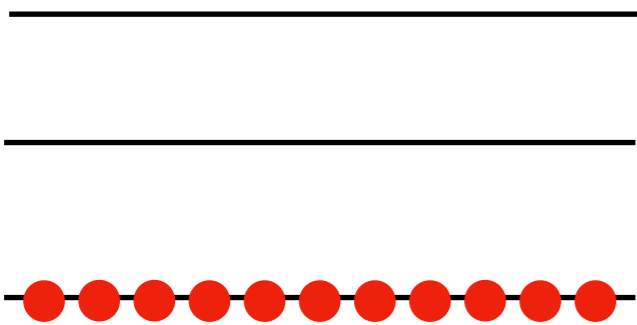
Bulk-boundary correspondence

— anomaly inflow —

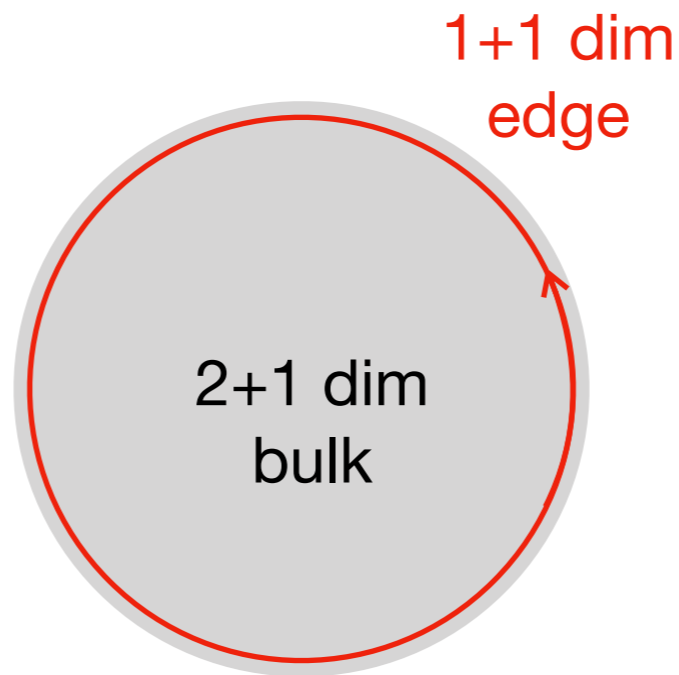
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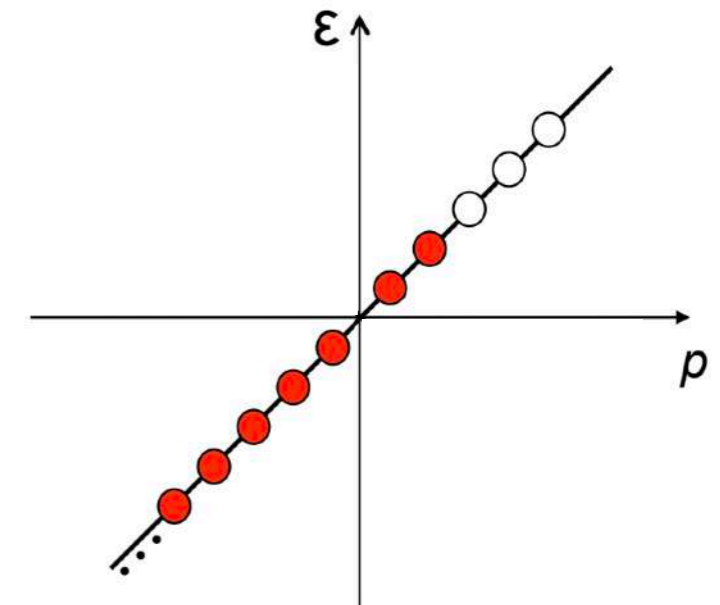


- Gauge invariant if no boundary
- Gauge dependent with boundary



1+1 dim edge
Chiral edge mode

$$H = v \int_{-\infty}^{\infty} dx \psi^* \left(-i \frac{\partial}{\partial x} \right) \psi.$$



Chiral anomaly

$$\partial_\mu j^\mu = \text{sign}(v) \frac{e^2 c}{4\pi \hbar} \epsilon^{\mu\nu} F_{\mu\nu}$$

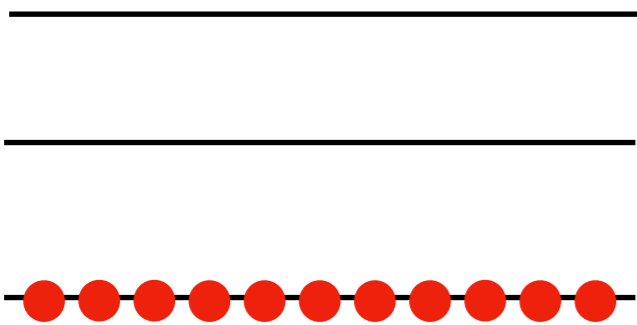
Bulk-boundary correspondence

— anomaly inflow —

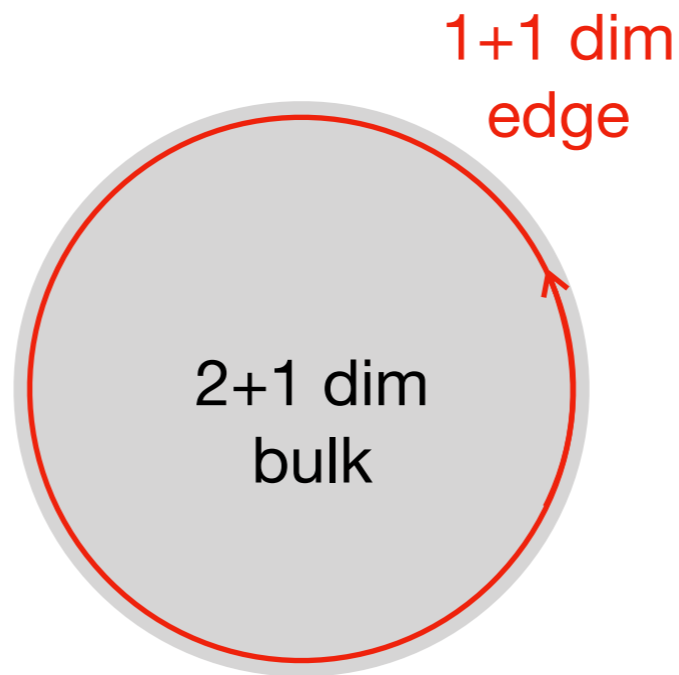
2+1 dim bulk:
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⋮



- Gauge invariant if no boundary
- Gauge dependent with boundary

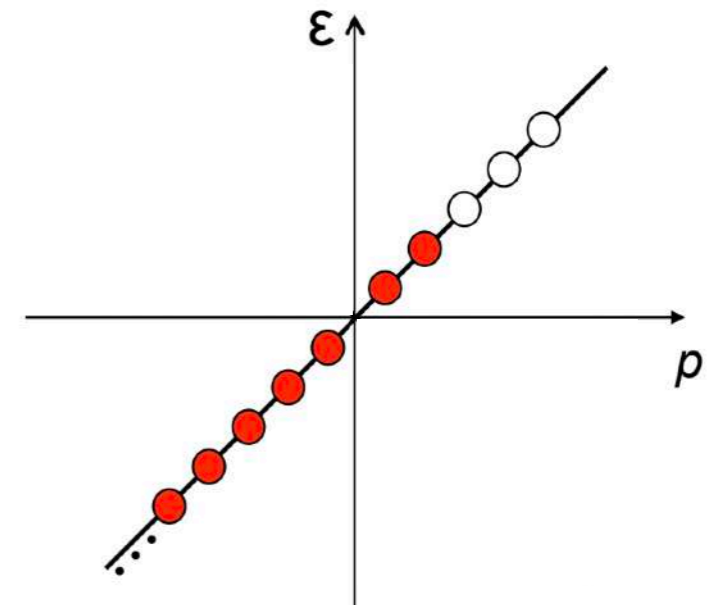


gauge dependence
cancels between
bulk and edge

robust against
decoration / perturbation
of surface

1+1 dim edge
Chiral edge mode

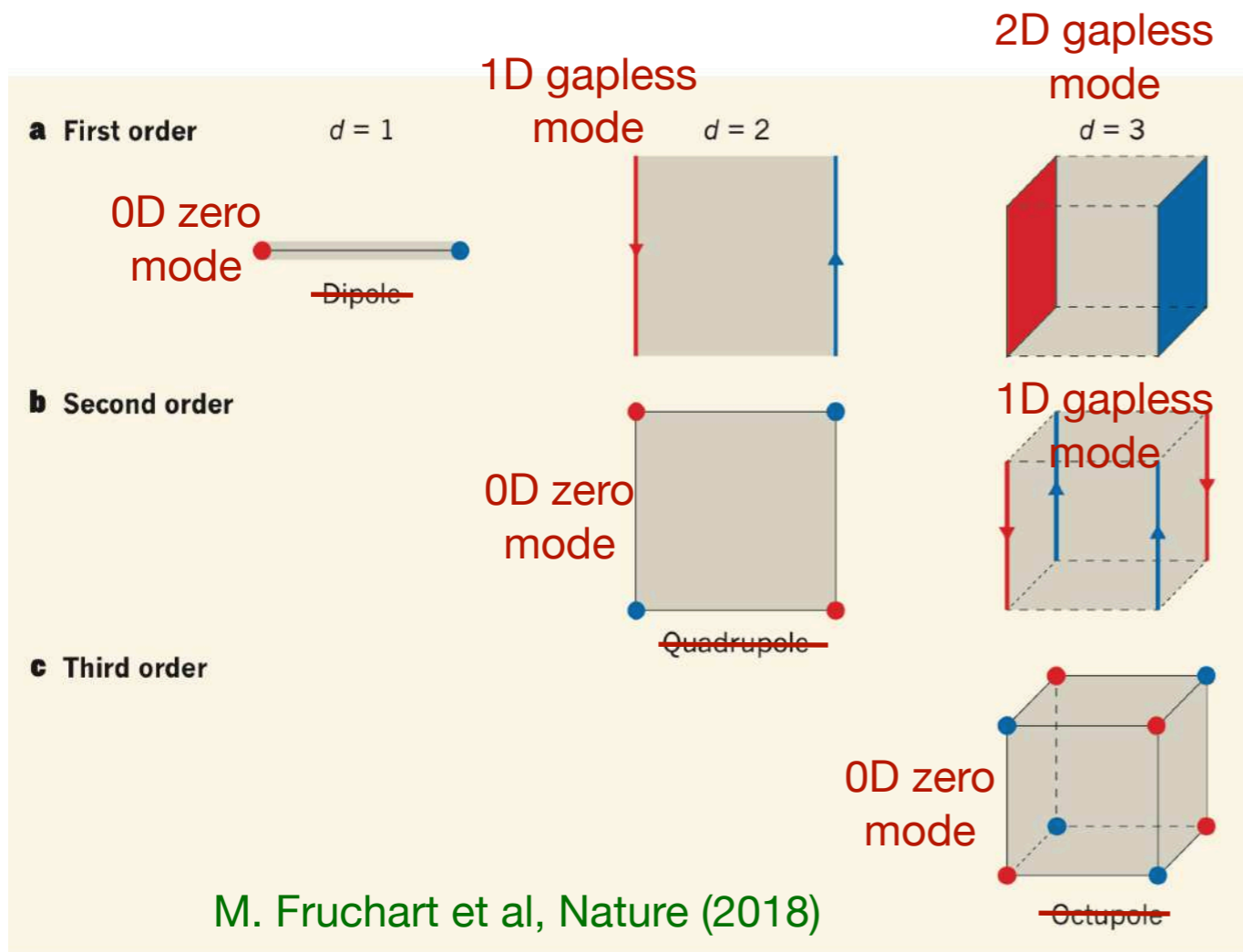
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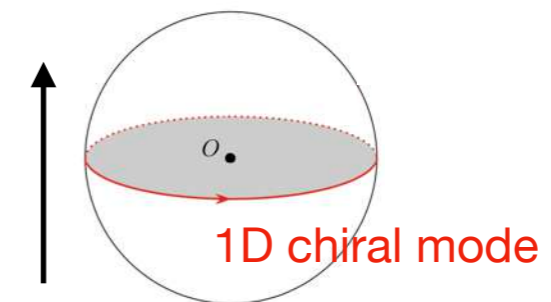
Chiral anomaly

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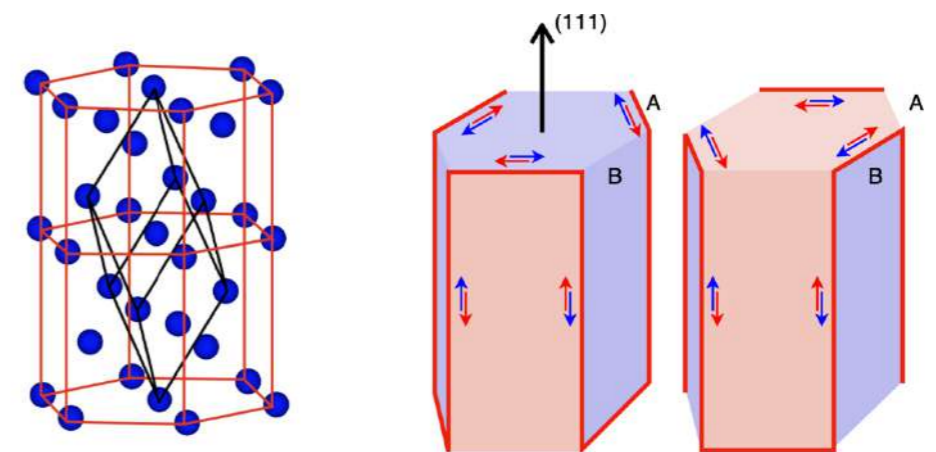
Bulk-boundary correspondence for higher-order topology



Inversion symmetric 3D topological insulator under magnetic field



Higher order topology in Bismuth

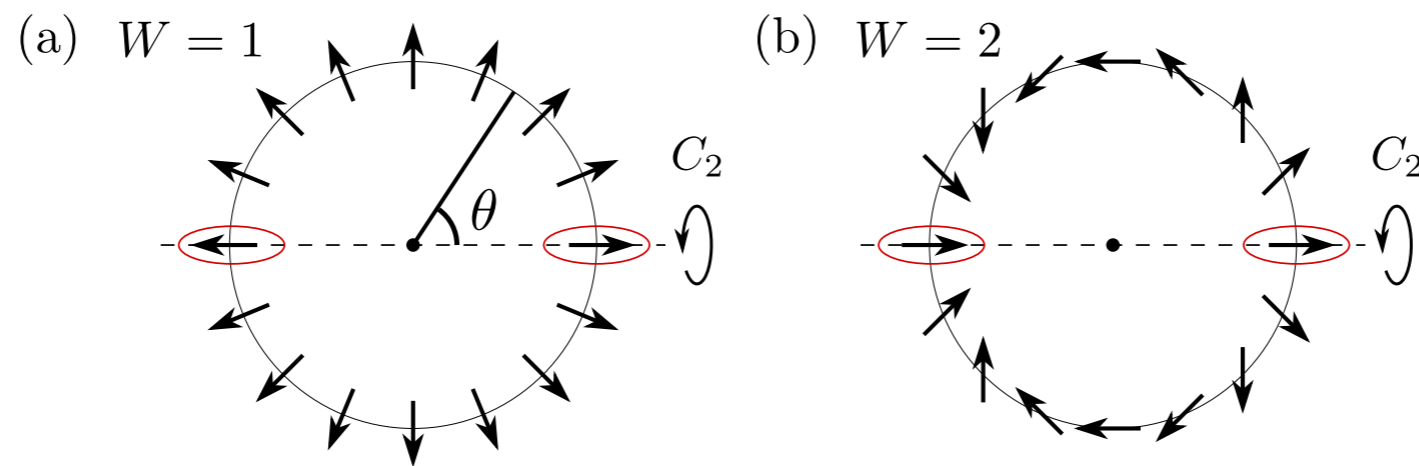


F. Schindler et al, Nature Physics (2018)
F. Schindler et al, Science Advances (2018)

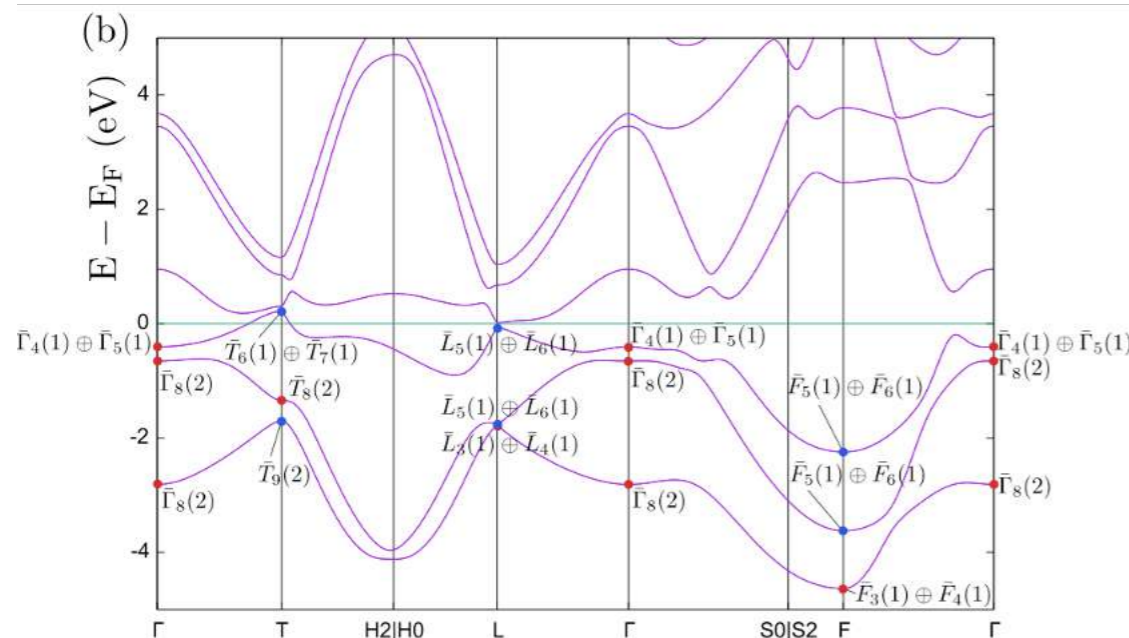
Boundary states can be localized to **corners** and **hinges** depending on the bulk topology.

Symmetry indicators of band topology

- A handy diagnosis of topology



- Similar relation holds in the band structure of electrons in solids



nature
COMMUNICATIONS

ARTICLE

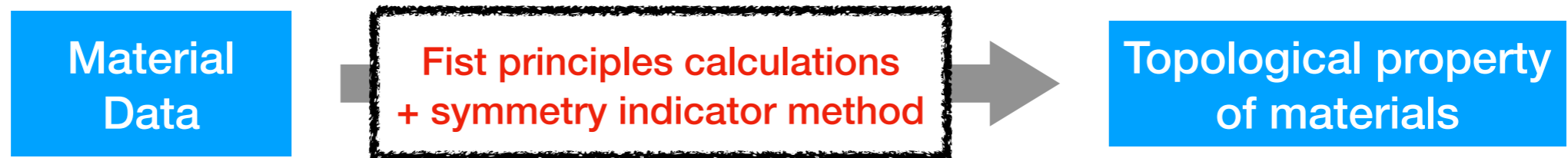
DOI: 10.1038/s41467-017-00133-2 OPEN

Symmetry-based indicators of band topology in the 230 space groups

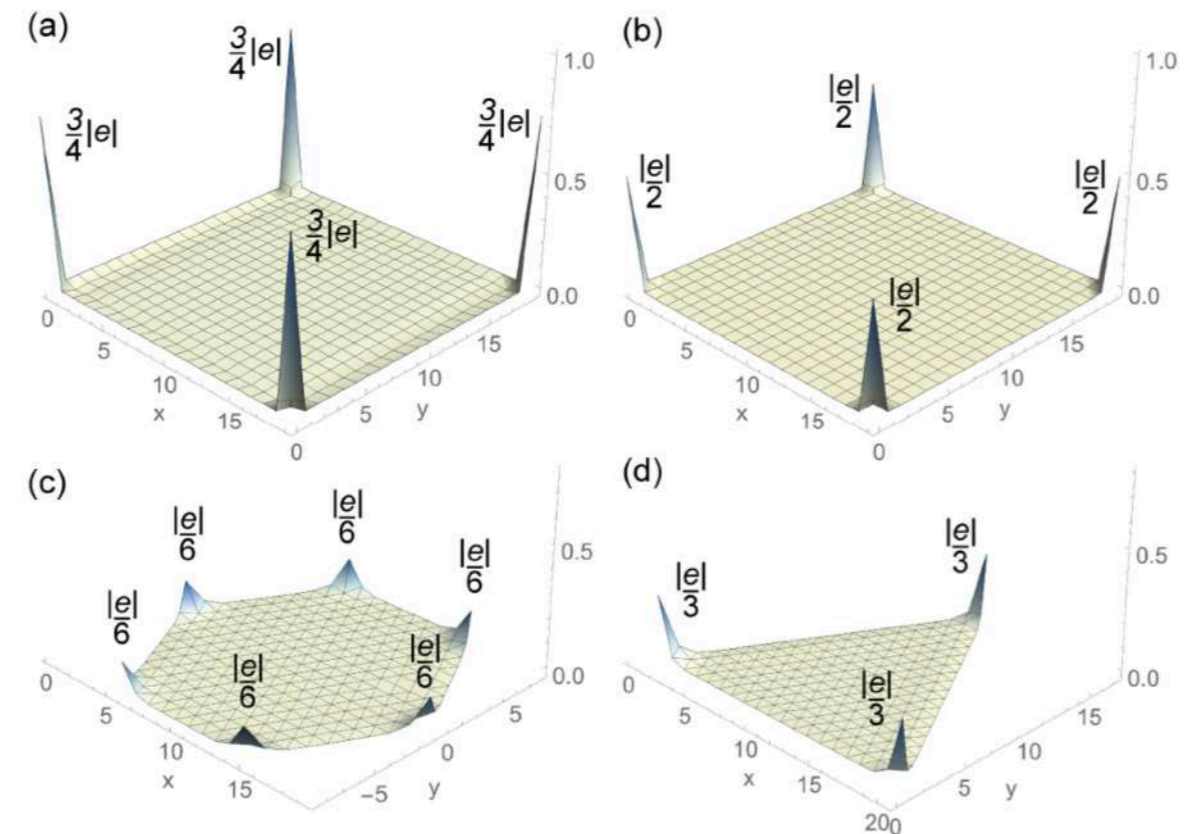
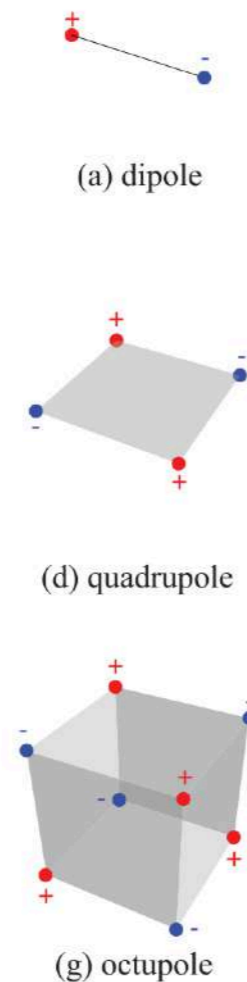
Hoi Chun Po^{1,2}, Ashvin Vishwanath^{1,2} & Haruki Watanabe³

A paradigm shift in material search

- Investigation of topological properties for *all* materials listed on database



Bulk-boundary correspondence of *trivial* insulators



Fractionally quantized
 → something topological

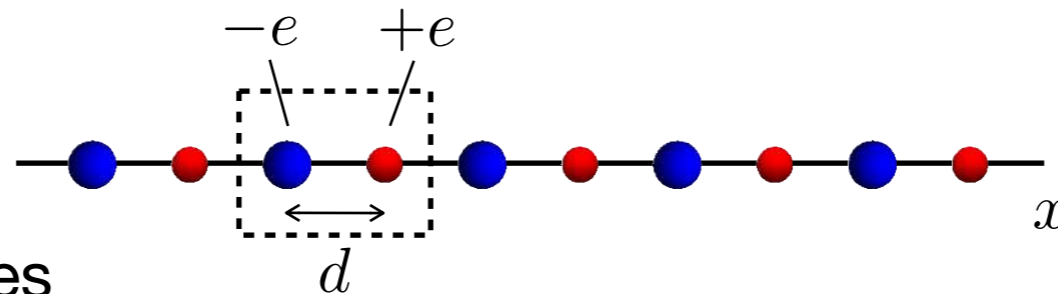
W. A. Benalcazar, B. A. Bernevig, T. L. Hughes,
 Science (2017) / PRB (2017)

W. A. Benalcazar, T. Li, T. L. Hughes,
 PRB (2019)

Bulk multipole moment implies boundary charges.
 Charges are “frozen” i.e., *not* degrees of freedom

Polarization and Edge charge

- Assume **U(1) symmetry** and **translation symmetry**

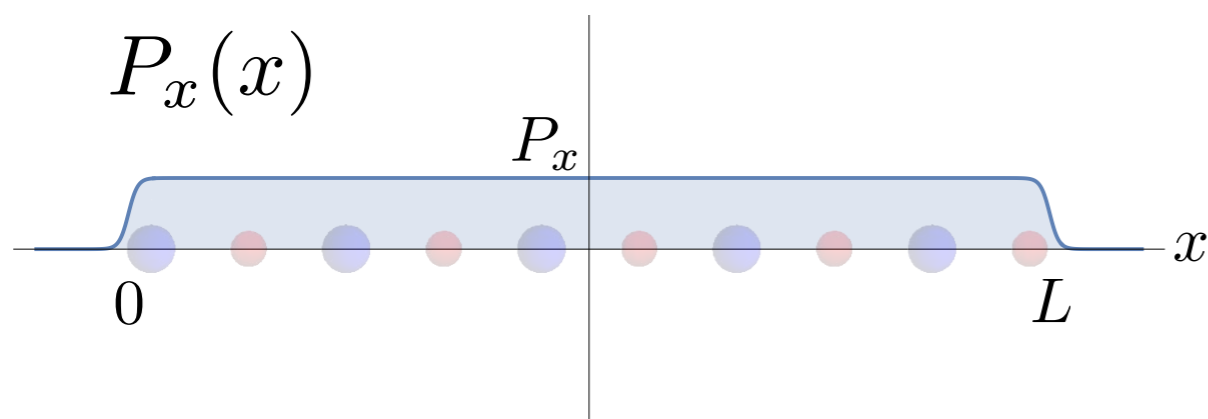


- For classical point charges

$$P_x^{(\text{classical})} = \frac{1}{a} \sum_{i \in \text{unit cell}} Q_i x_i = \frac{(-e)(x_0) + (+e)(x_0 + d)}{a} = e \frac{d}{a}$$

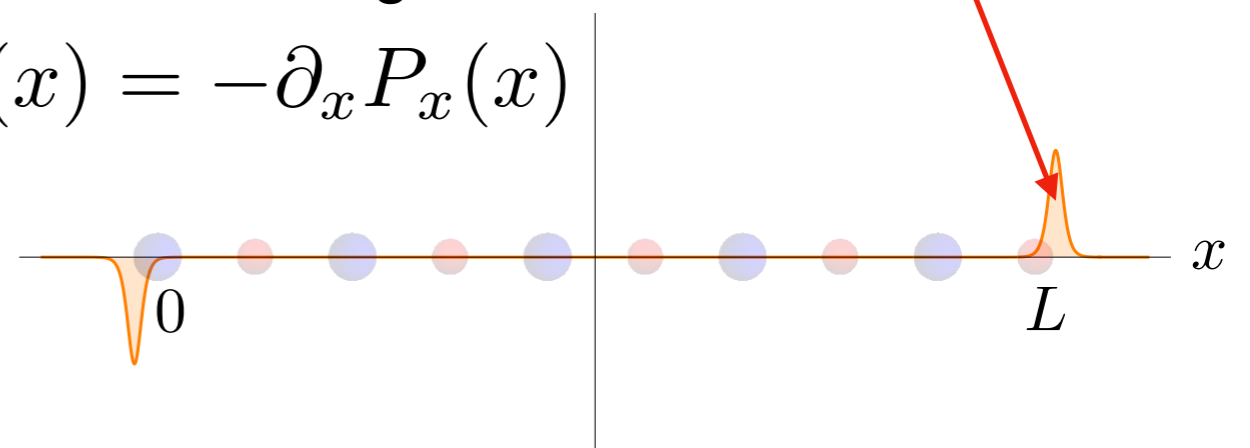
$$Q_{\text{edge}} \equiv - \int_{\text{edge}} dx \partial_x P(x) = P_x$$

Polarization



Polarization charge

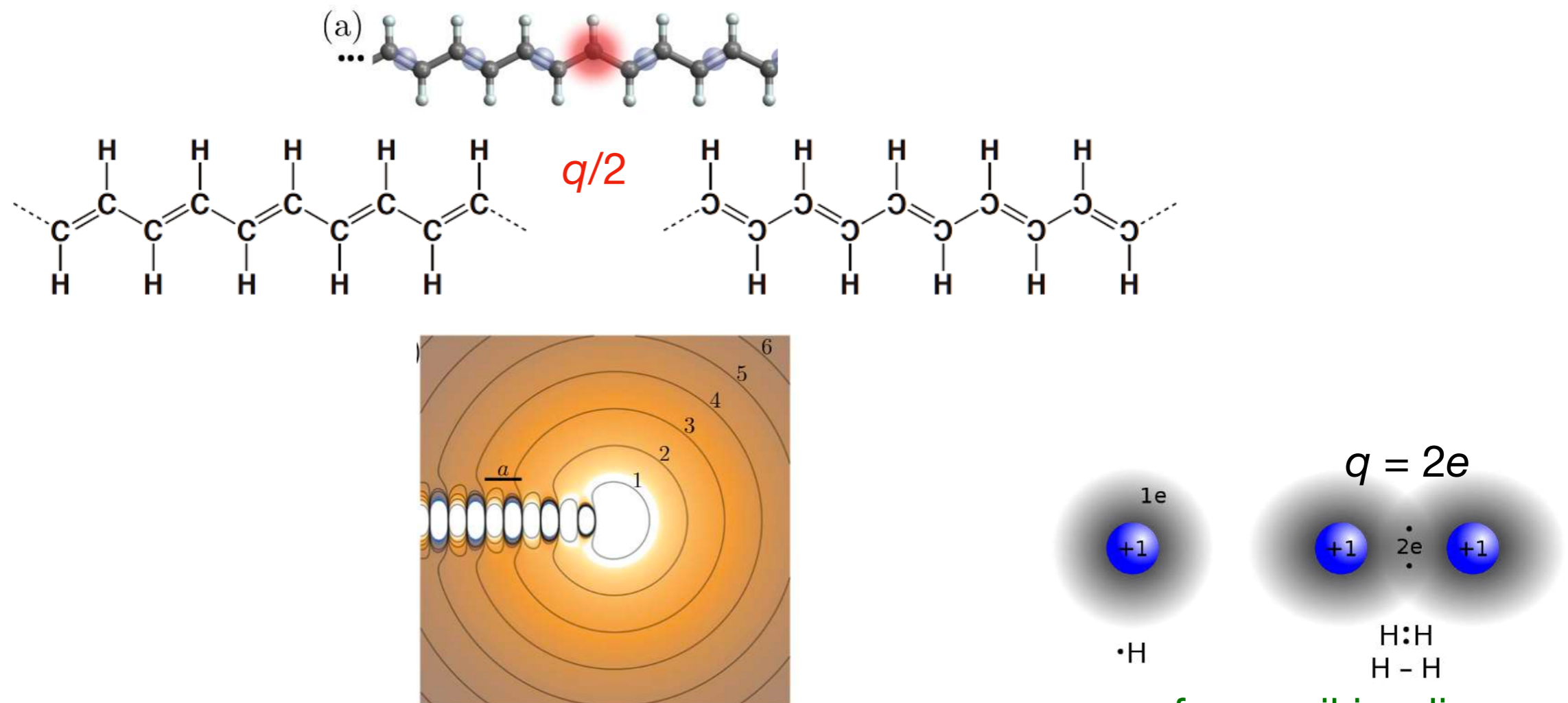
$$\rho(x) = -\partial_x P_x(x)$$



Edge charge is given by *bulk* polarization!

Solitons in polyacetylene

- R. Jackiw and C. Rebbi, "Solitons with fermion number 1/2," PRD (1976).
- W. P. Su, J. R. Schrieffer, and A. J. Heeger, "Solitons in polyacetylene," PRL (1979).
- A. J. Heeger, S. Kivelson, J. R. Schrieffer, and W. P. Su, "Solitons in conducting polymers," RMP (1988).

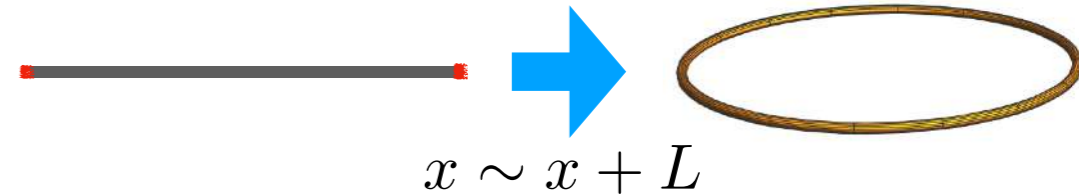


from: wikipedia

Formula of bulk polarization

“Modern theory”

- Periodic Boundary Condition (PBC): $\hat{c}_{x+L}^\dagger = \hat{c}_x^\dagger$
- Conserved U(1) charge and polarization operator



$$\hat{Q} \equiv \int_0^L dx \hat{\rho}(x) \quad \hat{P}_x \equiv \frac{1}{L} \int_0^L dx x \hat{\rho}(x)$$

\hat{P}_x is inconsistent with PBC.
 $\langle \hat{P}_x \rangle$ does not work in general!

- Berry phase formula

$$P_x = \langle \hat{P}_x \rangle + \frac{e}{2\pi} \gamma$$

Band insulators

$$\gamma = - \sum_{n \in \text{occ}} \int_0^{\frac{2\pi}{a}} dk u_{nk}^* i \partial_k u_{nk}$$

R. D. King-Smith, D. Vanderbilt PRB (1993)

$$u_{n, k + \frac{2\pi}{a}} = u_{nk}$$

$i \partial_k \sim x$

Interacting systems

$$\gamma = - \int_0^{2\pi} d\phi i \langle \phi | \partial_\phi | \phi \rangle$$

G. Ortiz, R. M. Martin, PRB (1994)
 HW, M. Oshikawa, PRX (2017)

Twisted Boundary Condition

$$\hat{c}_{x+L}^\dagger = e^{-i\phi} \hat{c}_x^\dagger \quad |\phi + 2\pi\rangle = |\phi\rangle$$

- Resta's formula

$$P_x = \frac{e}{2\pi} \text{Im} \log \langle e^{i2\pi \hat{P}_x / e} \rangle$$

R. Resta, PRL (1998)

We know how to compute the bulk P_x
 even for interacting systems!

Formula of bulk higher-order multipoles?

- Difficulties in generalizing the Berry phase formula

$$\sum_{n \in \text{occ}} \int_{\text{BZ}} \frac{dk_x}{2\pi} u_{nk_x}^* i \partial_{k_x} u_{nk_x} \rightarrow \sum_{n \in \text{occ}} \int_{\text{BZ}} \frac{d^2 k}{(2\pi)^2} u_{n\mathbf{k}}^* i \partial_{k_x} i \partial_{k_y} u_{n\mathbf{k}} \rightarrow \text{gauge dependent}$$

$i \partial_{k_x} i \partial_{k_y} \sim xy$ $u_{n\mathbf{k}} \rightarrow e^{i\theta_{\mathbf{k}}} u_{n\mathbf{k}}$

- Attempts in generalizing Resta's formula

$$\left\langle e^{2\pi i \int_0^{L_x} dx \frac{x}{L_x} \frac{\hat{\rho}(x)}{e}} \right\rangle \rightarrow \left\langle e^{2\pi i \int_0^{L_x} dx \int_0^{L_y} dy \frac{xy}{L_x L_y} \frac{\hat{\rho}(x,y)}{e}} \right\rangle$$

B. Kang, K. Shiozaki, G. Y. Cho, PRB (2019)

W. A. Wheeler, L. K. Wagner, T. L. Hughes, PRB (2019)

S. Ono, L. Trifunovic, HW, PRB (2019)

- Nested Wilson loop approach for band insulators (gives only the edge polarization.)

W. A. Benalcazar, B. A. Bernevig, T. L. Hughes, Science (2017) / PRB (2017)

- More direct generalization of the “modern theory”?

HW, S. Ono, PRB (2020)

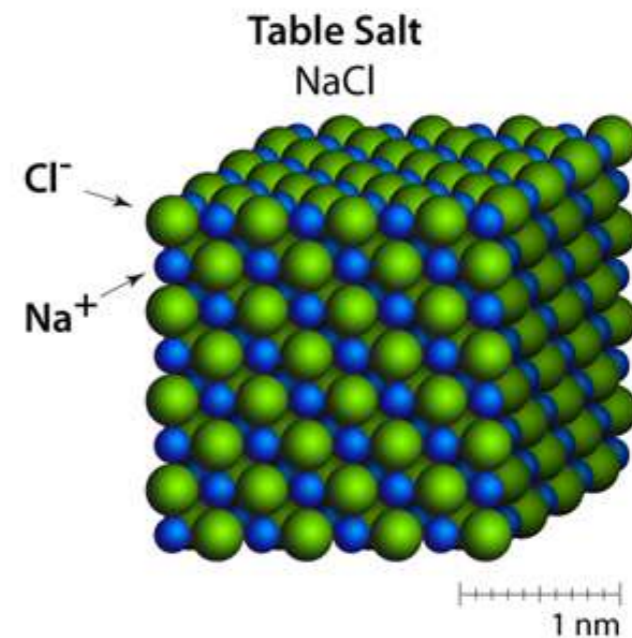
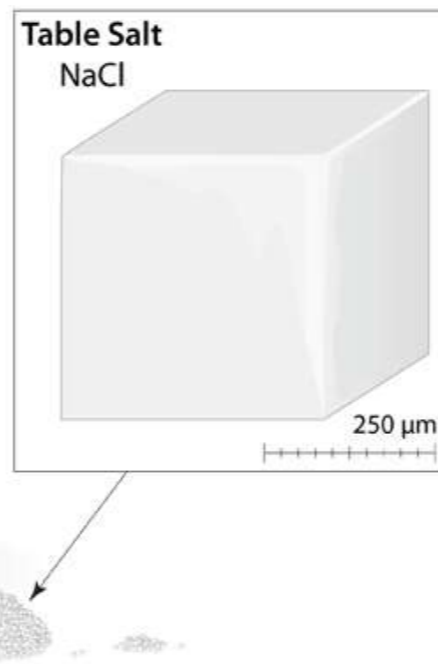
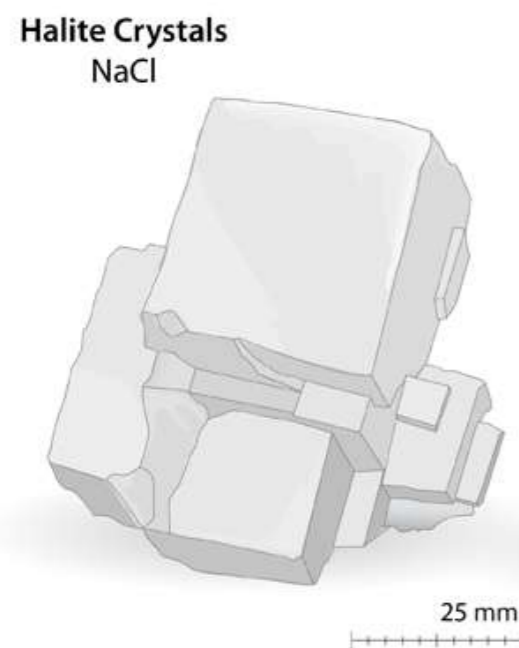
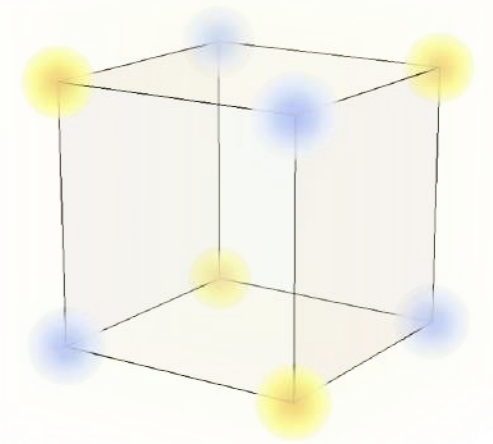
L. Trifunovic, PRR (2020)

S. H. Kooi, G. van Miert, C. Ortix, npj QM (2021)

S. Ren, I. Souza, D. Vanderbilt, PRB (2021)

Our goal

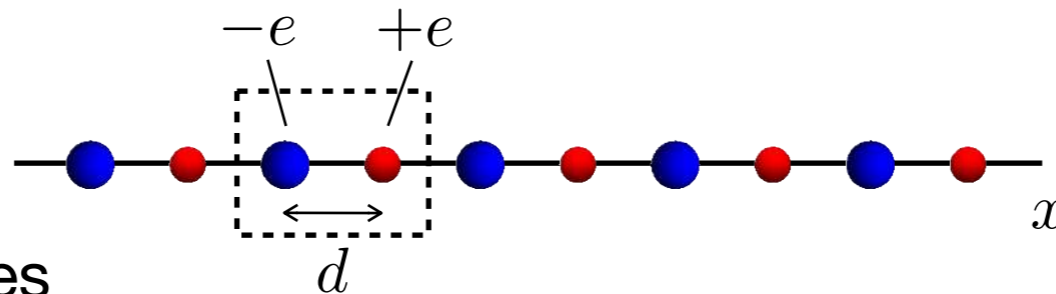
1. Give a general formulation of the bulk multipole moments
→ **Characterization of trivial phases of matter**
2. Clarify the relation to corner / hinges charges
3. Propose materials / experiments



Polarization in 1D systems

Polarization and Edge charge

- Assume **U(1) symmetry** and **translation symmetry**

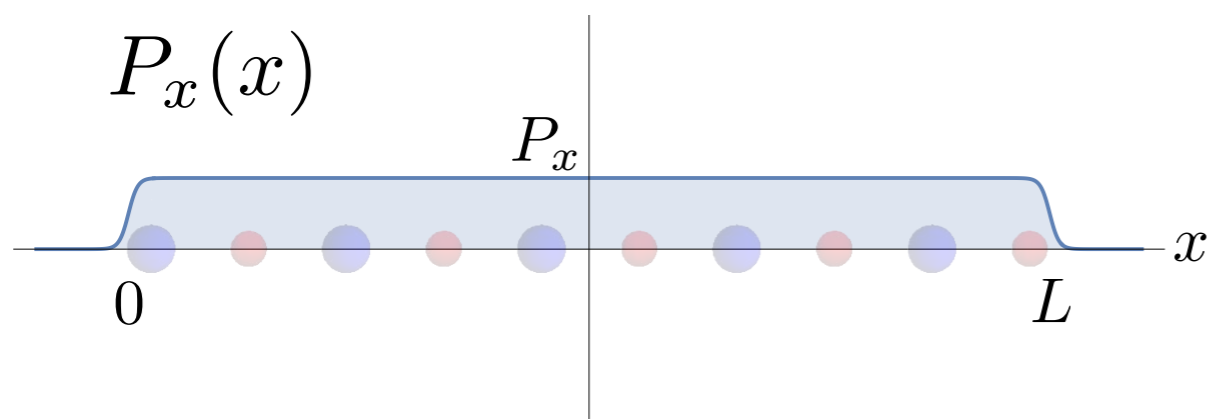


- For classical point charges

$$P_x^{(\text{classical})} = \frac{1}{a} \sum_{i \in \text{unit cell}} Q_i x_i = \frac{(-e)(x_0) + (+e)(x_0 + d)}{a} = e \frac{d}{a}$$

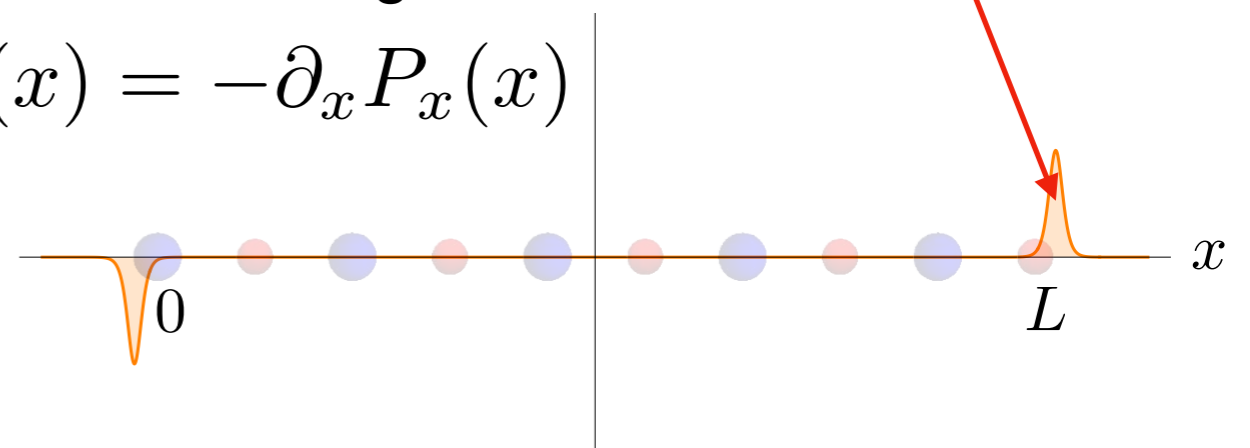
$$Q_{\text{edge}} \equiv - \int_{\text{edge}} dx \partial_x P(x) = P_x$$

Polarization



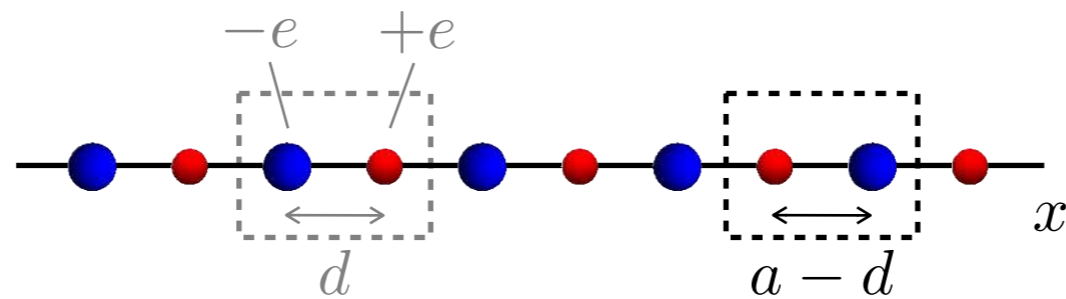
Polarization charge

$$\rho(x) = -\partial_x P_x(x)$$



Edge charge is given by *bulk* polarization!

Ambiguity of bulk polarization



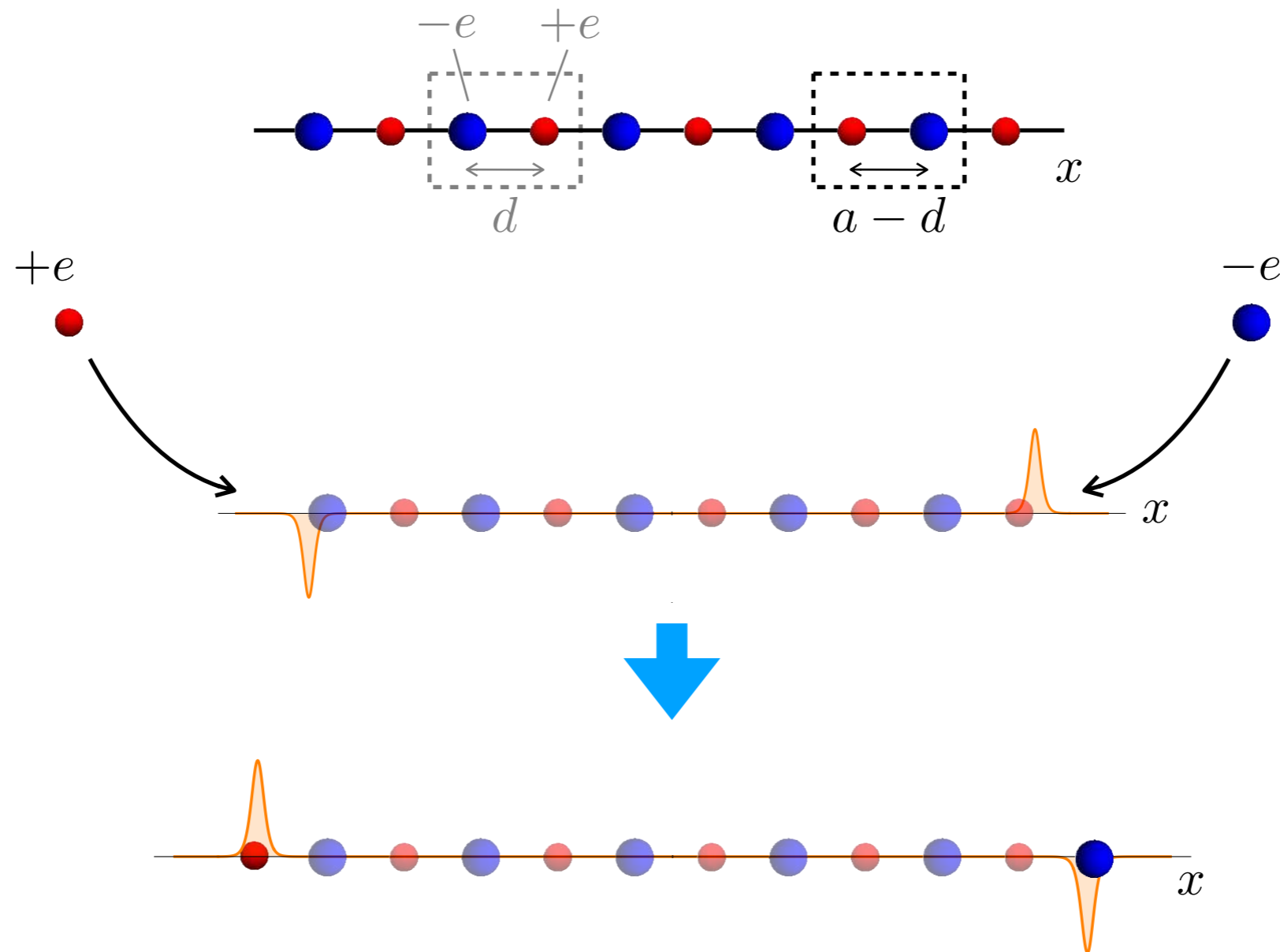
$$P_x^{(\text{classical})} = \frac{1}{a} \sum_{i \in \text{unit cell}} Q_i x_i = \frac{(-e)(x_0) + (+e)(x_0 + d)}{a} = e \frac{d}{a}$$



$$P_x^{(\text{classical})} = \frac{1}{a} \sum_{i \in \text{unit cell}} Q_i x_i = \frac{(-e)(x_0) + (+e)(x_0 + d - a)}{a} = e \frac{d}{a} - e$$

**Bulk polarization has an integer ambiguity.
(Choice of unit cell)**

Ambiguity of edge charge



**Edge charge also has an integer ambiguity.
(Choice of edge termination & decoration)**

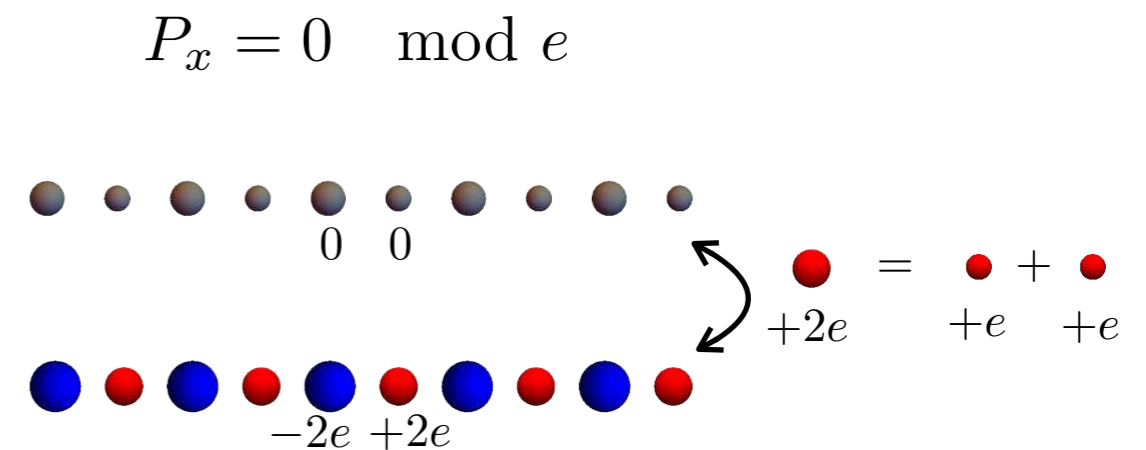
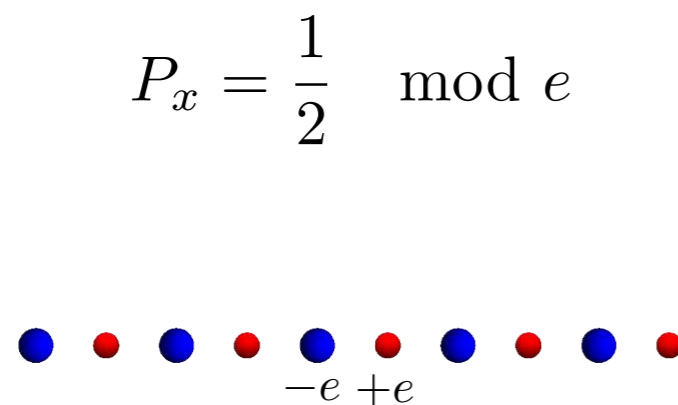
Quantization under symmetry

- Assume **inversion symmetry** ($x \rightarrow -x$) in addition to **U(1)** and **translation**.
- Inversion symmetry flips the sign of polarization \rightarrow quantization to 0 or $e/2$.

$$-P_x = P_x \pmod{e} \quad \rightarrow \quad P_x = 0 \text{ or } \frac{1}{2}e \pmod{e}$$

- There are at least two phases \rightarrow trivial phases are not unique!

Y. Fuji, F. Pollmann, M. Oshikawa, PRL (2015)
 H. C. Po, A. Vishwanath, [HW](#), Nature Comm (2017)
 + many other works in the context of TCI

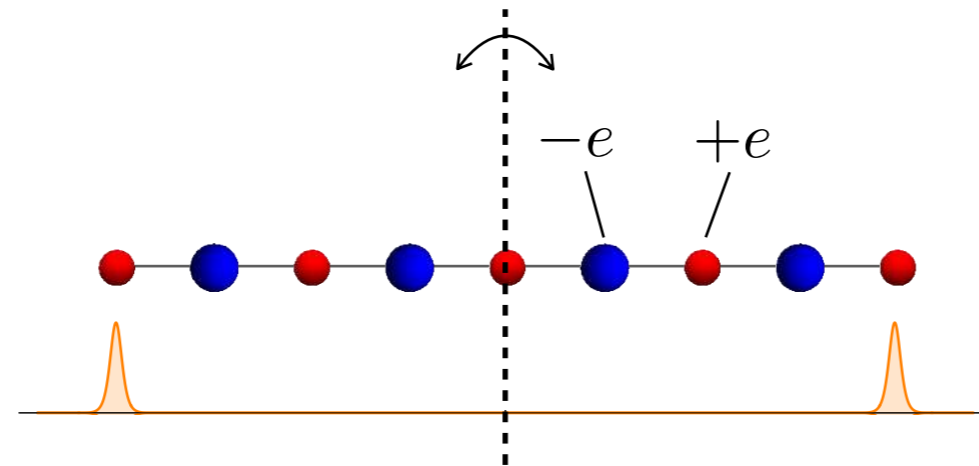


The U(1) charge $Q \pmod{2e}$ at the inversion center is a topological invariant.

“Filling anomaly”

- Sometimes **charge neutrality** and **point-group symmetry** cannot be simultaneously respected.

W. A. Benalcazar, T. Li, T. L. Hughes,
PRB (2019)



$$Q_{\text{tot}} = +e$$

$$Q_{\text{edge}} = \frac{1}{2} Q_{\text{tot}} \pmod{e}$$

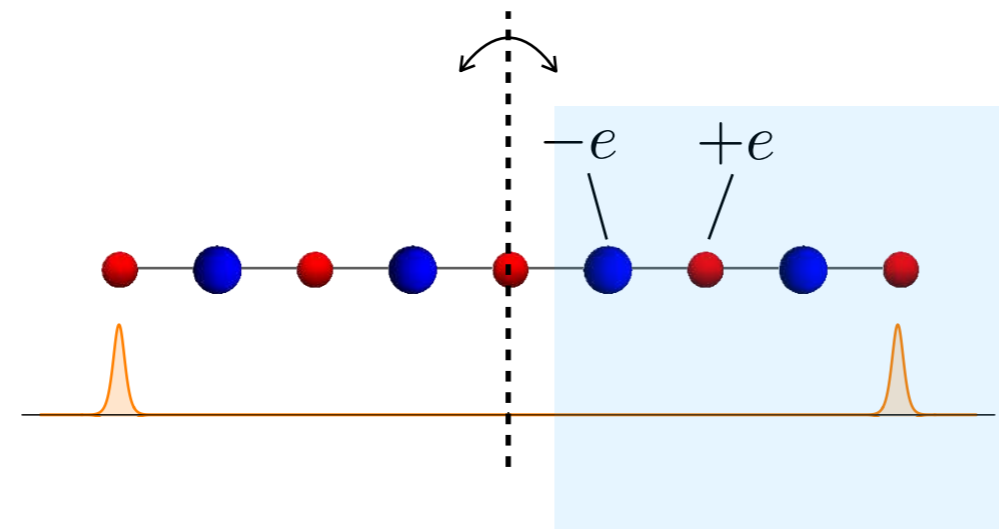
Note:

1. This formula assumes charges are localized to edges.
2. Termination has to be designed carefully.

“Filling anomaly”

- Sometimes **charge neutrality** and **point-group symmetry** cannot be simultaneously respected.

W. A. Benalcazar, T. Li, T. L. Hughes,
PRB (2019)

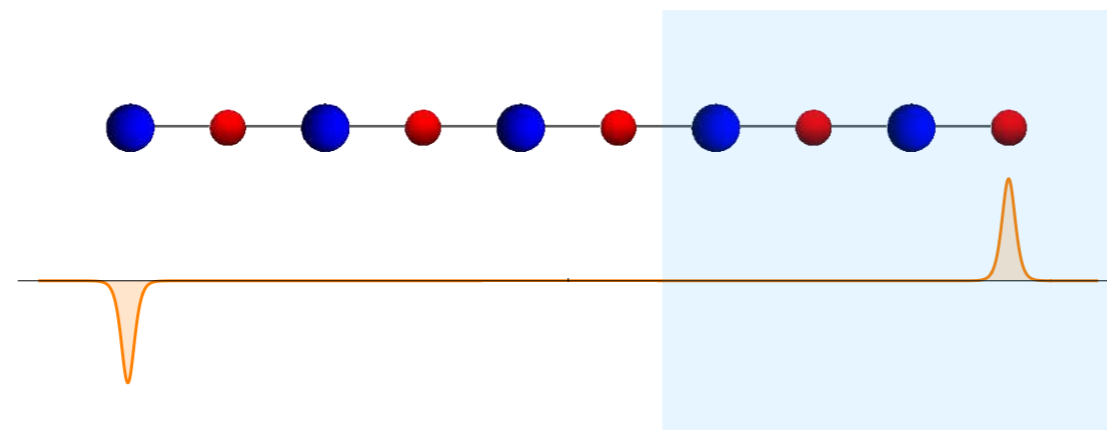


$$Q_{\text{tot}} = +e$$

$$Q_{\text{edge}} = \frac{1}{2} Q_{\text{tot}} \pmod{e}$$

Note:

- This formula assumes charges are localized to edges.
- Termination has to be designed carefully.



$$Q_{\text{tot}} = 0$$

Corner charge is a local property.
Not affected by the other edge

Definition of the edge charge

- Conserved charge of the U(1) symmetry:

$$\hat{Q} = \int dx \hat{\rho}(x)$$

- Microscopic charge density:

$$\rho^{(\text{micro})}(x) = \langle \hat{\rho}(x) \rangle$$

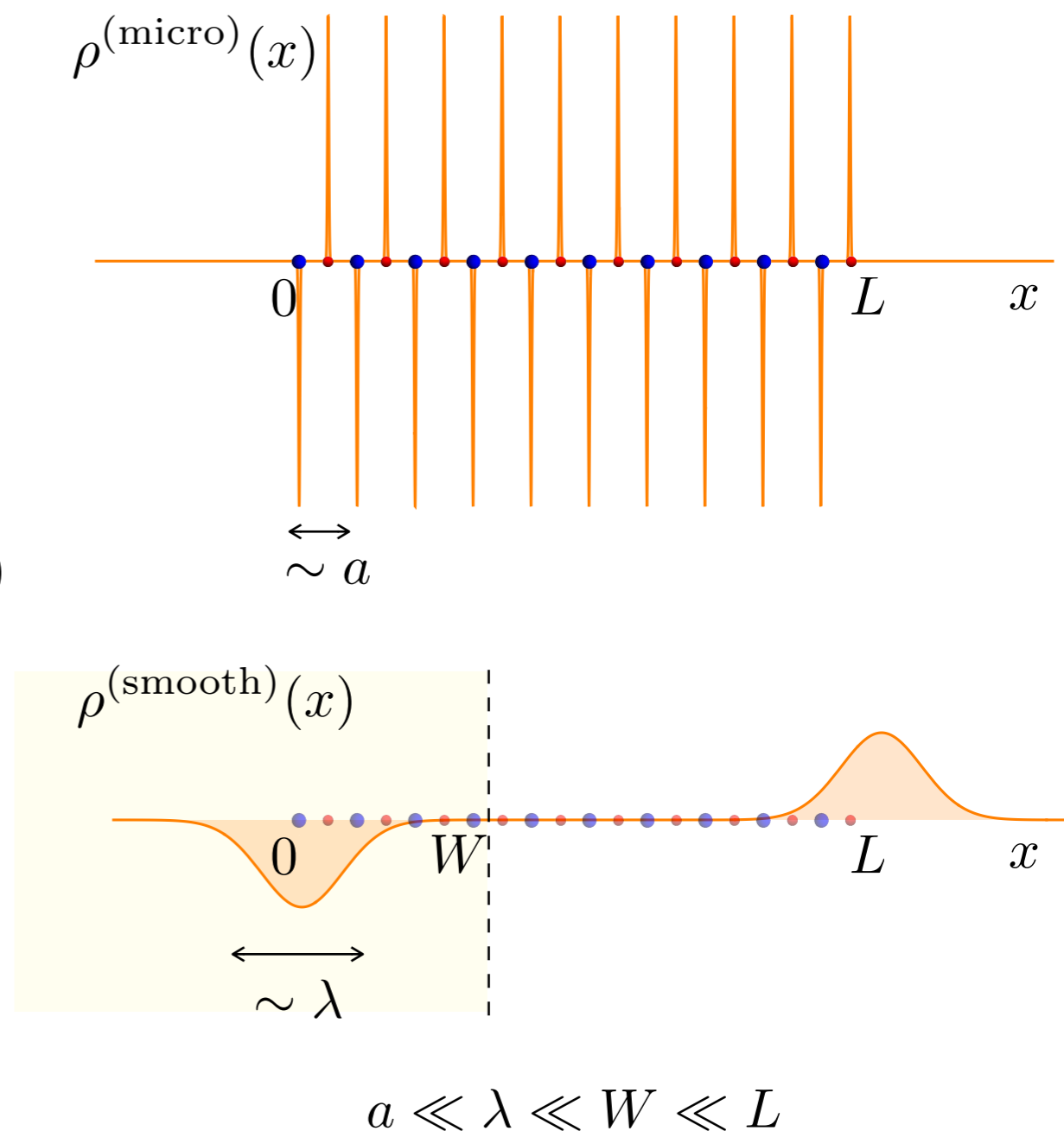
- Coarse-grained charge density:

$$\rho^{(\text{smooth})}(x) \equiv \int_{-\infty}^{\infty} dx' g(x-x') \rho^{(\text{micro})}(x')$$

$$g(x) = \frac{1}{\sqrt{2\pi\lambda^2}} e^{-\frac{1}{2\lambda^2}x^2}$$

- Definition of edge charge:

$$Q_{\text{edge}} \equiv \int_{-\infty}^W dx \rho^{(\text{smooth})}(x)$$



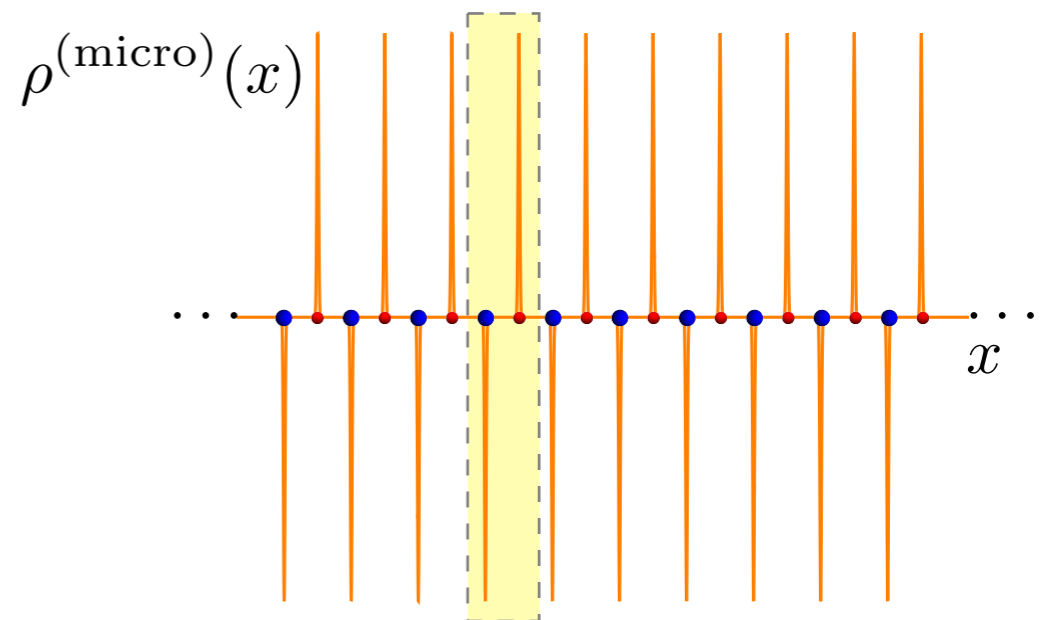
(Definition of the bulk polarization)

- Translation invariance
→ a repetition unit of charge density

$$\rho^{(\text{micro})}(x) = \sum_{n=-\infty}^{+\infty} \rho_0(x - na)$$

$\rho_0(x)$ is not unique. $\rho_0(x) \rightarrow 0$ when $|x| \gg a$

We require $\int_{-\infty}^{\infty} dx \rho_0(x) = 0$

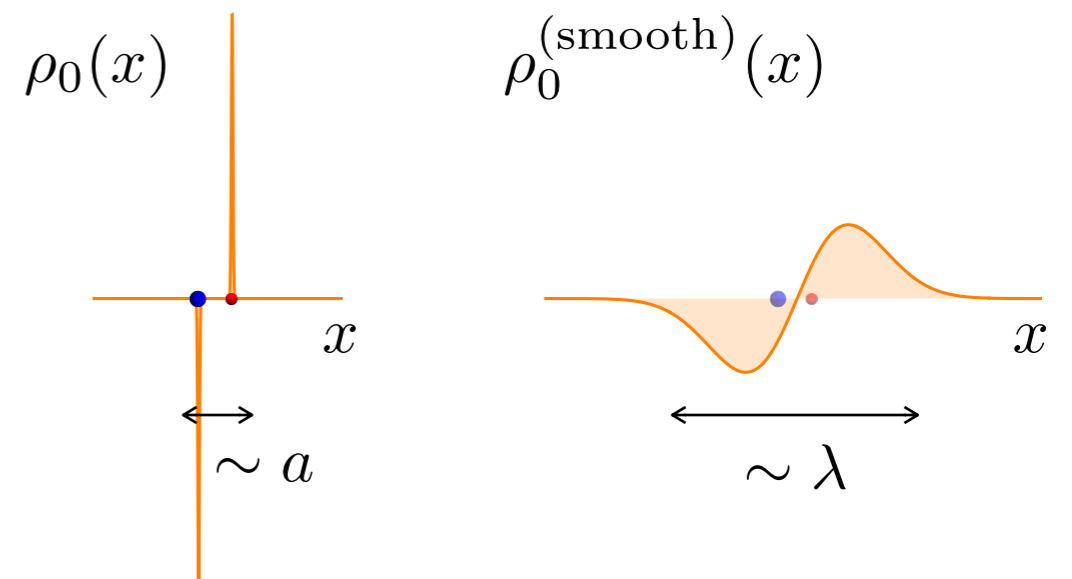


- Definition of bulk polarization

$$P_x \equiv \frac{1}{a} \int_{-\infty}^{\infty} dx x \rho_0(x)$$

$$\left(= \frac{1}{a} \int_{-\infty}^{\infty} dx x \rho_0^{(\text{smooth})}(x) \right)$$

$$\rho_0^{(\text{smooth})}(x) \equiv \int_{-\infty}^{\infty} dx' g(x - x') \rho_0(x)$$

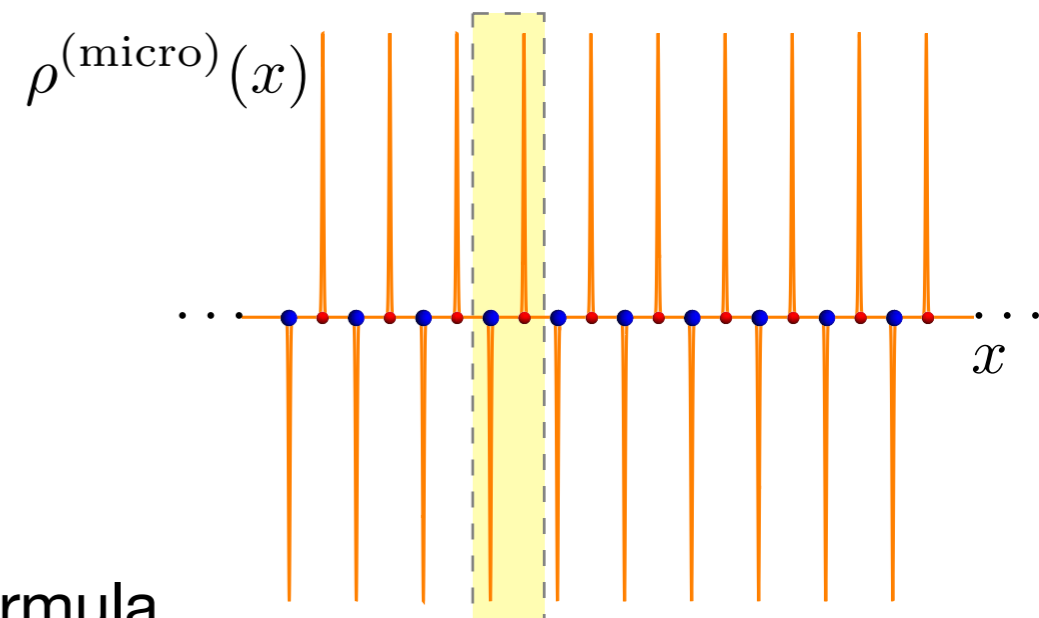


(Definition of the bulk polarization)

- For band insulators, $\rho_0(x)$ is given by Wannier function

$$\rho_0^{(\text{el})}(x) = -\frac{ea}{L} \sum_R \sum_{n \in \text{occ}} |w_{n,i}(R)|^2 \delta(x - R - x_i)$$

$$w_{n,i}(R) \sim \int_0^{\frac{2\pi}{a}} \frac{dk}{2\pi} u_{nk,i} e^{ikR}$$



- Our expression of P_x reduces to the Berry phase formula

$$\begin{aligned} P_x &\equiv \frac{1}{a} \int_{-\infty}^{\infty} dx x \rho_0(x) \\ &= \langle \hat{P}_x \rangle - e \sum_{n \in \text{occ}} \int_0^{\frac{2\pi}{a}} \frac{dk}{2\pi} u_{nk}^* i \partial_k u_{nk} \end{aligned}$$

(Proof of the bulk-edge correspondence)

Infinite system

$$\rho^{(\text{micro})}(x) = \sum_{n=-\infty}^{+\infty} \rho_0(x - na)$$



Semi-infinite system

$$\rho^{(\text{micro})}(x) = \sum_{n=0}^{+\infty} \rho_0(x - na)$$

$$\begin{aligned} \rho^{(\text{smooth})}(x) &\equiv \int_{-\infty}^{\infty} dx' g(x - x') \rho^{(\text{micro})}(x) \\ &= \int_{-\infty}^{\infty} dx' g(x - x') \sum_{n=0}^{\infty} \rho_0(x - na) = \sum_{n=0}^{\infty} \rho_0^{(\text{smooth})}(x - na) \\ &\underset{(\lambda \gg a)}{\simeq} \frac{1}{a} \int_0^{\infty} dx' \rho_0^{(\text{smooth})}(x - x') = \frac{1}{a} \int_{-\infty}^x dx'' \rho_0^{(\text{smooth})}(x'') \end{aligned}$$

$$\begin{aligned} Q_{\text{edge}} &\equiv \int_{-\infty}^W dx \rho^{(\text{smooth})}(x) \\ &\simeq \frac{1}{a} \int_{-\infty}^W dx \int_{-\infty}^x dx' \rho_0^{(\text{smooth})}(x') = \frac{1}{a} \int_{-\infty}^W dx' \int_{x'}^W dx \rho_0^{(\text{smooth})}(x') \\ &= \frac{1}{a} \int_{-\infty}^W dx' (W - x') \rho_0^{(\text{smooth})}(x') \simeq -\frac{1}{a} \int_{-\infty}^{\infty} dx' x' \rho_0^{(\text{smooth})}(x') = -P_x \end{aligned}$$

**Higher order multipoles
in higher D systems**

2D: Quadrupole moment and corner charge

- Charge density

$$\rho^{(\text{micro})}(\mathbf{r}) = \sum_{n_i \geq 0} \rho_0(\mathbf{r} - \sum_{i=1}^d n_i \mathbf{a}_i).$$

- The total charge in the region R

$$Q_R = \int_R d^d r \rho^{(\text{smooth})}(\mathbf{r}) = W_1 \sigma_2 + W_2 \sigma_1 + Q_{\text{corner}}$$

- Surface charge density

$$\sigma_i = - \int_{\mathbb{R}^d} d^d r \rho_0(\mathbf{r}) P_i(\mathbf{r})$$

$$P_i(\mathbf{r}) \equiv \mathbf{b}_i \cdot \mathbf{r} \quad \mathbf{a}_i \cdot \mathbf{b}_j = \delta_{ij}$$

- Corner charge

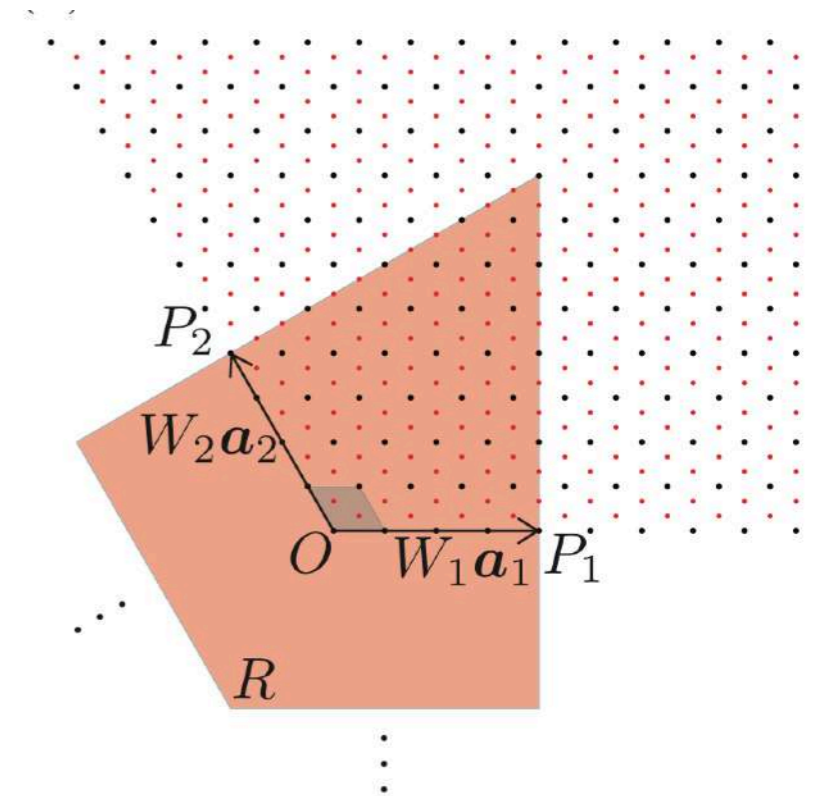
$$Q_{\text{corner}} = \int_{\mathbb{R}^d} d^d r \rho_0(\mathbf{r}) Q_{12}(\mathbf{r})$$

$$Q_{12}(\mathbf{r}) \equiv (\mathbf{b}_1 \cdot \mathbf{r})(\mathbf{b}_2 \cdot \mathbf{r}) + \frac{\mathbf{a}_2 \cdot \mathbf{a}_1}{2a_2^2} (\mathbf{b}_1 \cdot \mathbf{r})^2 + \frac{\mathbf{a}_1 \cdot \mathbf{a}_2}{2a_1^2} (\mathbf{b}_2 \cdot \mathbf{r})^2$$

$$= \frac{1}{a_1 a_2} \left(\frac{x^2 - y^2}{2} \cos \theta + xy \sin \theta \right).$$

$$\mathbf{a}_1 = a_1(1, 0)$$

$$\mathbf{a}_2 = a_2(\cos \theta, \sin \theta)$$



3D: Octupole moment and corner/hinge charge

- Charge density

$$\rho^{(\text{micro})}(\mathbf{r}) = \sum_{n_i \geq 0} \rho_0(\mathbf{r} - \sum_{i=1}^d n_i \mathbf{a}_i).$$

- The total charge in the region R

$$Q_R = \int_R d^d r \rho^{(\text{smooth})}(\mathbf{r}) = \sum_{i=1}^3 S_i \sigma_i + \sum_{i=1}^3 W_i \lambda_i + Q_{\text{corner}}$$

- Hinge charge density

$$\lambda_3 = \int_{\mathbb{R}^d} d^d r \rho_0(\mathbf{r}) Q_{12}(\mathbf{r})$$

$$Q_{12}(\mathbf{r}) \equiv (\mathbf{b}_1 \cdot \mathbf{r})(\mathbf{b}_2 \cdot \mathbf{r}) + \frac{\mathbf{a}_1 \cdot \mathbf{b}_1 \times \mathbf{a}_3}{2\mathbf{a}_2 \cdot \mathbf{b}_1 \times \mathbf{a}_3} (\mathbf{b}_1 \cdot \mathbf{r})^2 + \frac{\mathbf{a}_2 \cdot \mathbf{b}_2 \times \mathbf{a}_3}{2\mathbf{a}_1 \cdot \mathbf{b}_2 \times \mathbf{a}_3} (\mathbf{b}_2 \cdot \mathbf{r})^2$$

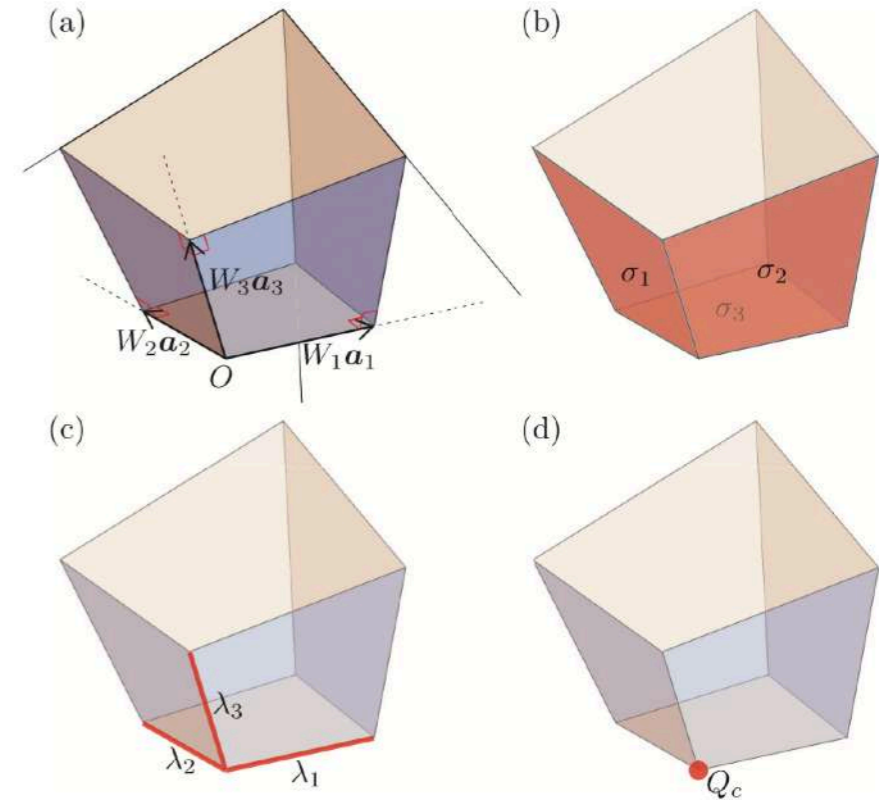
- Corner charge

$$Q_{\text{corner}} = \int_{\mathbb{R}^d} d^d r \rho_0(\mathbf{r}) Q_{123}(\mathbf{r})$$

$$c_{ij} \equiv -\frac{\mathbf{a}_i \cdot \mathbf{a}_j}{a_i^2} \quad r_i \equiv \mathbf{b}_i \cdot \mathbf{r}$$

$$O_{123}(\mathbf{r}) = r_1 r_2 r_3 - \frac{1}{2}(c_{23} r_3^2 + c_{32} r_2^2) r_1 - \frac{1}{2}(c_{31} r_1^2 + c_{13} r_3^2) r_2 - \frac{1}{2}(c_{12} r_2^2 + c_{21} r_1^2) r_3$$

$$+ \frac{c_{23} c_{31}^2 + 2c_{21} c_{31} + c_{32} c_{21}^2}{6(1 - c_{23} c_{32})} r_1^3 + \frac{c_{31} c_{12}^2 + 2c_{32} c_{12} + c_{13} c_{32}^2}{6(1 - c_{31} c_{13})} r_2^3 + \frac{c_{12} c_{23}^2 + 2c_{13} c_{23} + c_{21} c_{13}^2}{6(1 - c_{12} c_{21})} r_3^3$$



(Ambiguities in bulk multipole moment)

- $\rho_0(x)$ is not unique!

$$\rho^{(\text{micro})}(\mathbf{r}) \equiv \langle \hat{\rho}(\mathbf{r}) \rangle = \sum_{n_i \in \mathbb{Z}} \rho_0(\mathbf{r} - \sum_{i=1}^d n_i \mathbf{a}_i) \quad \left\{ \begin{array}{l} \int_{\mathbb{R}^d} d^d r \rho_0(\mathbf{r}) = 0 \\ \rho_0(\mathbf{r}) \rightarrow 0 \quad \text{when } |\mathbf{x}| \gg a \end{array} \right.$$

$$\rho_0^{(\text{el})}(x) = -\frac{ea}{L} \sum_R \sum_{n \in \text{occ}} |w_{n,i}(R)|^2 \delta(x - R - x_i) \quad w_{n,i}(R) \sim \int_0^{\frac{2\pi}{a}} \frac{dk}{2\pi} u_{nk,i} e^{ikR}$$

- Wannier center has only integer ambiguity
→ fractional part of polarization is well-defined.
But spread of Wannier function is gauge-dependent.

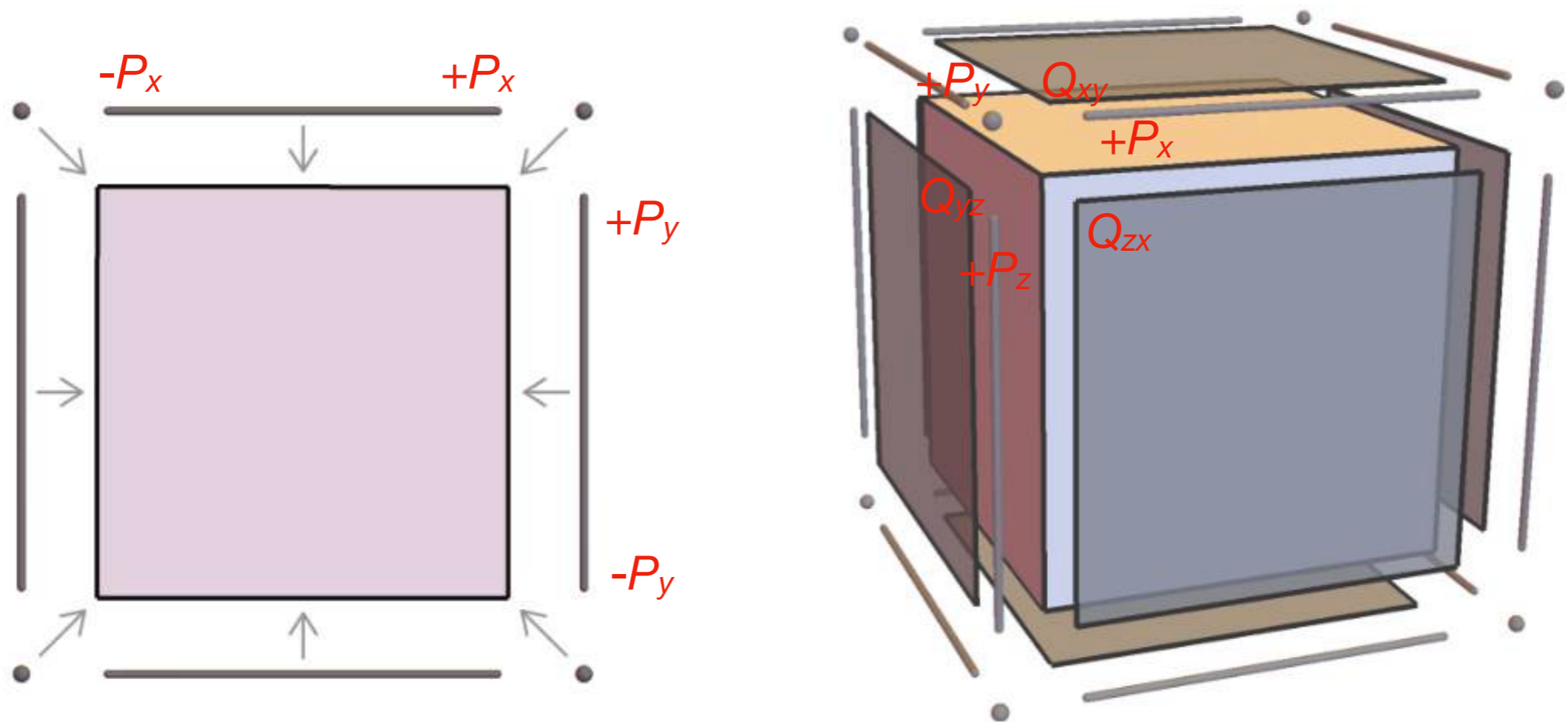
- Higher moments depend on the specific choice of $\rho_0(\mathbf{r})$

$$\int_{\mathbb{R}^d} d^d r \rho_0(\mathbf{r}) r_i \quad \int_{\mathbb{R}^d} d^d r \rho_0(\mathbf{r}) r_i r_j \quad \int_{\mathbb{R}^d} d^d r \rho_0(\mathbf{r}) r_i r_j r_k$$

Ambiguities in corner/hinger charge

$$Q_{\text{corner}} \rightarrow Q_{\text{corner}} + P_x + P_y$$

$$Q_{\text{corner}} \rightarrow Q_{\text{corner}} + P_x + P_y + P_z + Q_{xy} + \dots$$



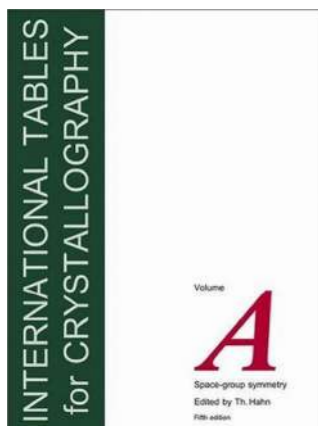
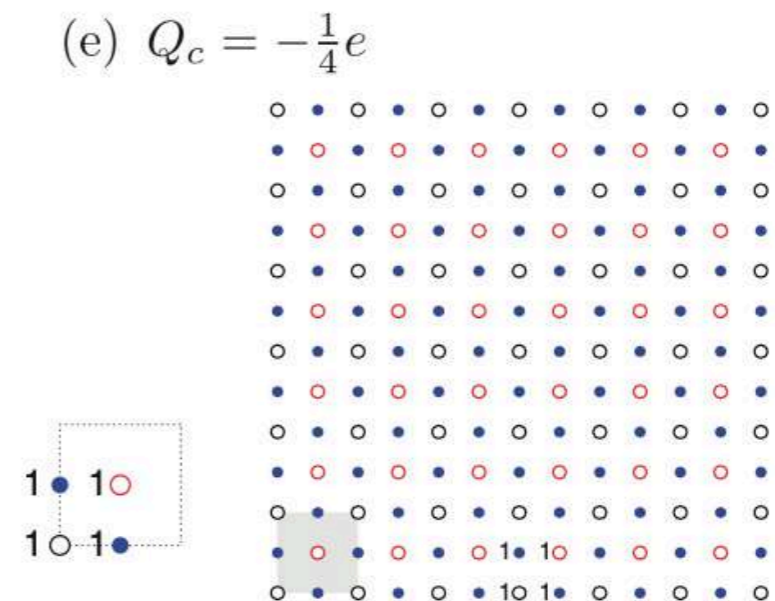
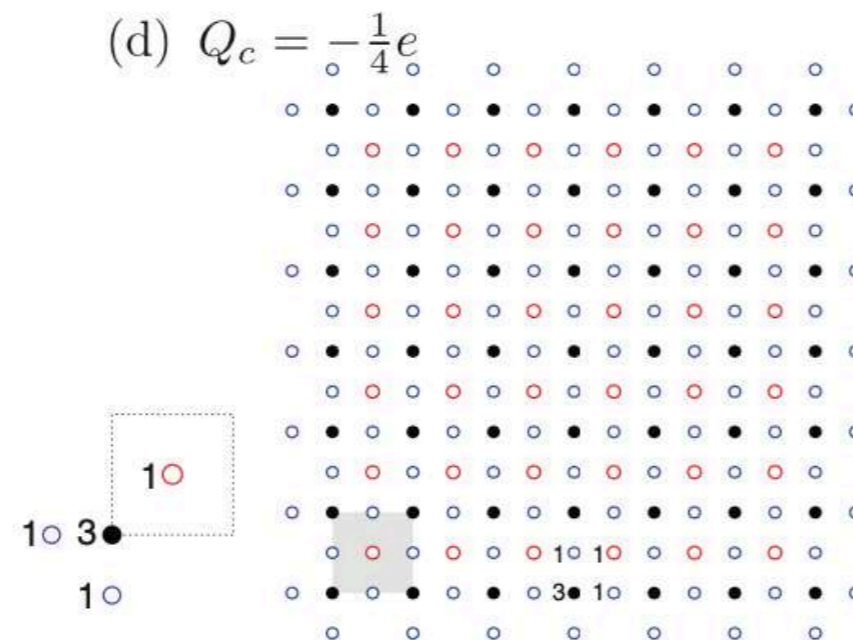
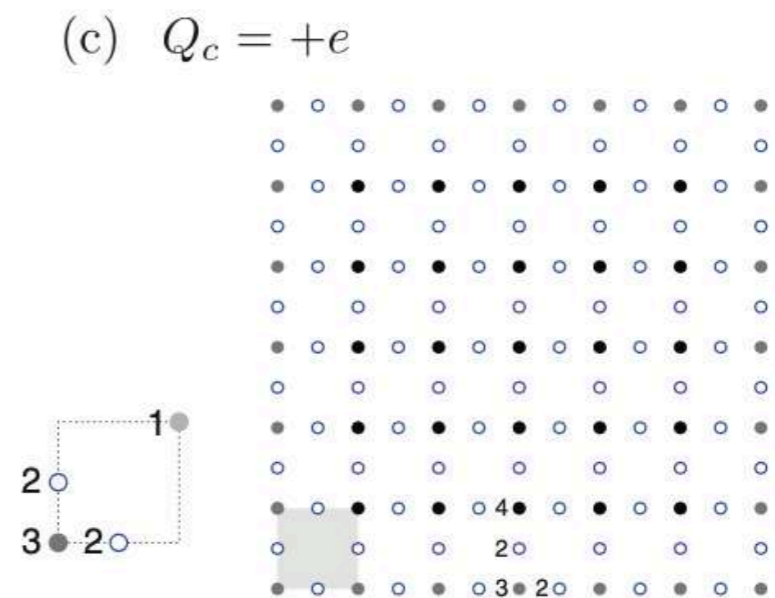
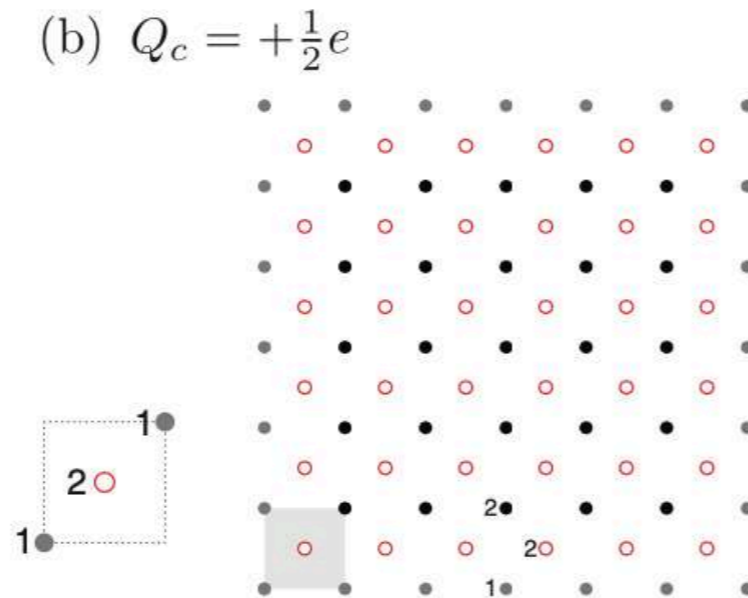
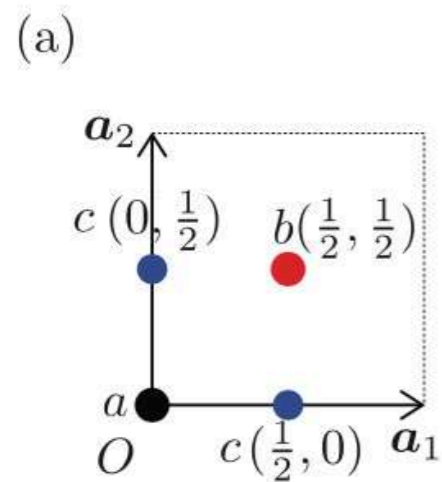
Corner charge not well-defined.
 (Choice of termination & decoration)
Point group symmetry is required!!

2D system under C_4 rotation

$$Q_{\text{corner}} = \int_{\mathbb{R}^d} d^d r \rho_0(\mathbf{r}) Q_{12}(\mathbf{r}) = \frac{1}{4} q_a = \frac{1}{4} q_b \pmod{e}$$

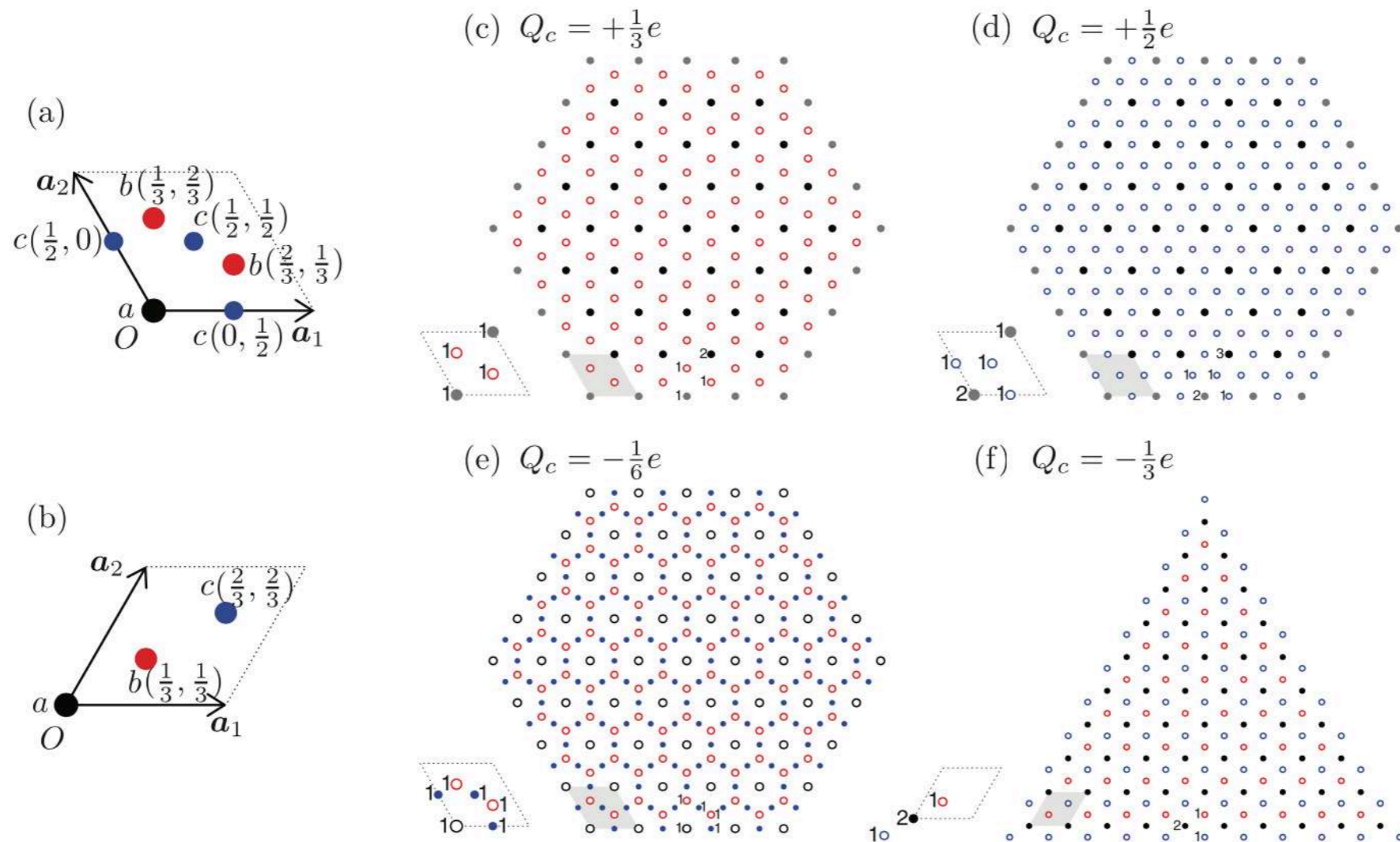
The U(1) charge on high-symmetry points

Classification of high-symmetry points: (special) Wyckoff position



2D system under C_3 or C_6 rotation

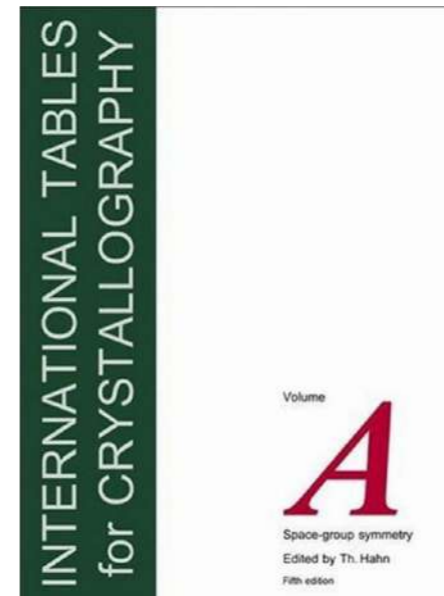
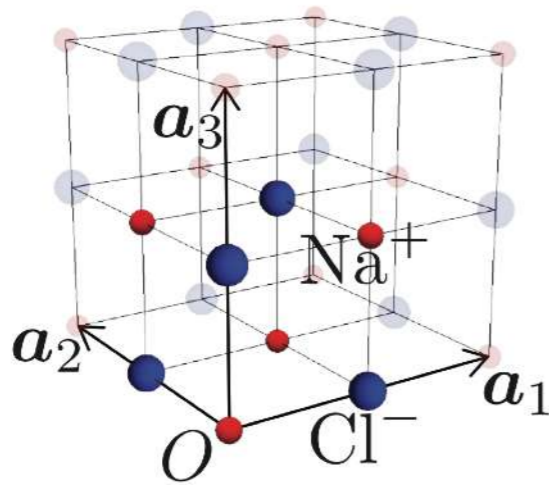
$$Q_{\text{corner}} = \int_{\mathbb{R}^d} d^d r \rho_0(\mathbf{r}) Q_{12}(\mathbf{r}) = \begin{cases} \frac{1}{6} q_a = \frac{2}{3} q_b + \frac{1}{2} q_c \pmod{e} & (n = 6) \\ \frac{1}{3} q_a = \frac{1}{3} q_b = \frac{1}{3} q_c \pmod{e} & (n = 3) \end{cases}$$



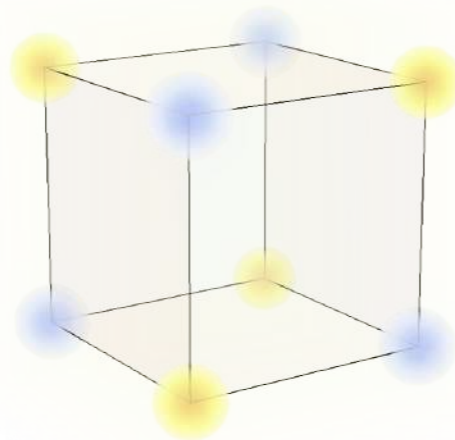
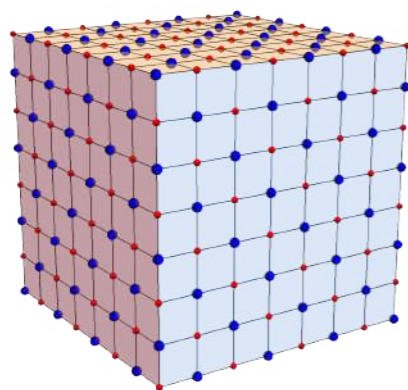
The $U(1)$ charge $Q \pmod{ne}$ at a C_n rotation axis is topological invariant.
Our results implies $Q_{\text{corner}} = Q/n \pmod{e}$

3D system under O_h symmetry

$$Q_{\text{corner}} = \int_{\mathbb{R}^d} d^d r \rho_0(\mathbf{r}) Q_{123}(\mathbf{r}) = \frac{1}{8} q_a = \frac{1}{8} q_b \pmod{\frac{1}{4} e}$$



CONTINUED		No. 221		$Pm\bar{3}m$	
Generators selected (1), (4,10), (6,14), (8,14), (11), (7), (9), (13), (15)		Conditions		Restriction conditions	
Position				A, B, C, D, E, F, G, H, I, J, K, L, M, N, O, P, Q, R, S, T, U, V, W, X, Y, Z	
Multiplicity				A, B, C, D, E, F, G, H, I, J, K, L, M, N, O, P, Q, R, S, T, U, V, W, X, Y, Z	
Wyckoff position				A, B, C, D, E, F, G, H, I, J, K, L, M, N, O, P, Q, R, S, T, U, V, W, X, Y, Z	
Site symmetry				A, B, C, D, E, F, G, H, I, J, K, L, M, N, O, P, Q, R, S, T, U, V, W, X, Y, Z	
48	48×1	(1) 1,1,1	(2) 1,1,1	(3) 1,1,1	(4) 1,1,1
24	24×2	1,1,1	1,1,1	1,1,1	1,1,1
12	12×4	1,1,1	1,1,1	1,1,1	1,1,1
6	6×8	1,1,1	1,1,1	1,1,1	1,1,1
3	3×16	1,1,1	1,1,1	1,1,1	1,1,1
2	2×24	1,1,1	1,1,1	1,1,1	1,1,1
1	1×48	1,1,1	1,1,1	1,1,1	1,1,1



3	d	$4/m\bar{3}m$	$\frac{1}{2}, 0, 0$	$0, \frac{1}{2}, 0$	$0, 0, \frac{1}{2}$
3	c	$4/m\bar{3}m$	$0, \frac{1}{2}, \frac{1}{2}$	$\frac{1}{2}, 0, \frac{1}{2}$	$\frac{1}{2}, \frac{1}{2}, 0$
1	b	$m\bar{3}m$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$		
1	a	$m\bar{3}m$	$0, 0, 0$		

The U(1) charge $Q \pmod{2e}$ at a O_h center is topological invariant.

Our formula is $Q_{\text{corner}} = Q/8 \pmod{e/4}$.

Filling anomaly

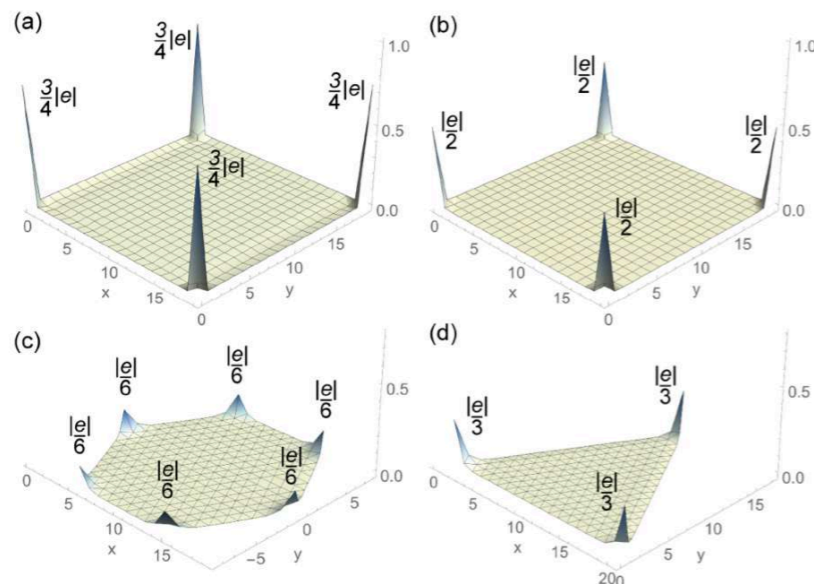
- Simple formula for the corner charge

$$Q_{\text{corner}} = Q_{\text{tot}} / N_{\text{corner}}$$

W. A. Benalcazar, T. Li, T. L. Hughes,
PRB (2019)

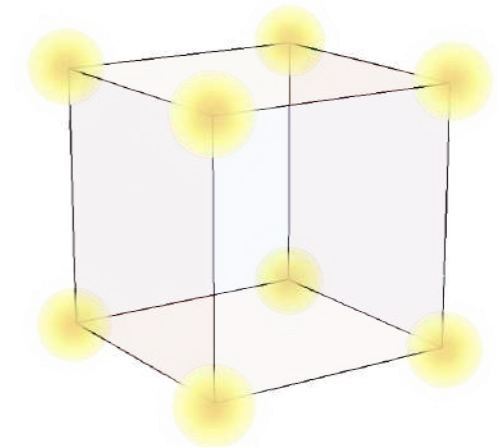
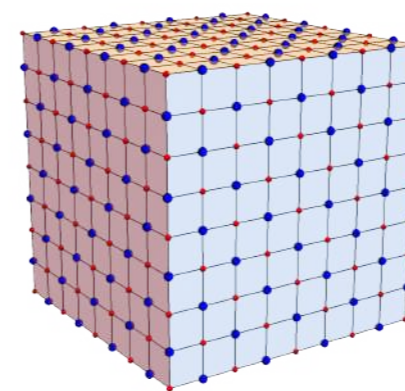
Q_{tot} = The total U(1) charge in the system

N_{corner} = The number of point-group related corners



$$Q_{\text{tot}} = +e, \quad Q_{\text{corner}} = \frac{1}{n}e \pmod{e}$$

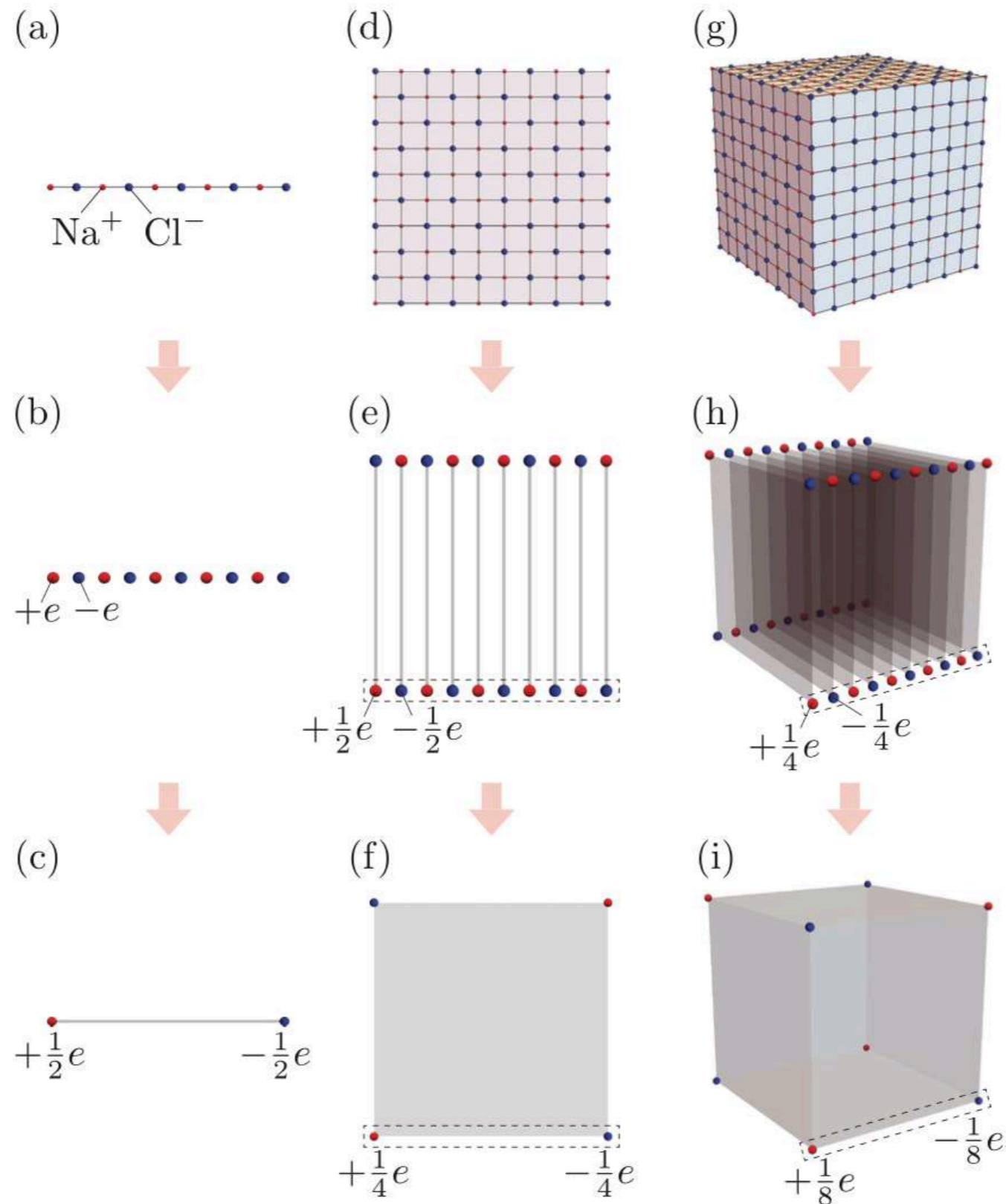
W. A. Benalcazar, T. Li, T. L. Hughes,
PRB (2019)



$$Q_{\text{tot}} = +e, \quad Q_{\text{corner}} = \frac{1}{8}e \pmod{\frac{1}{4}e}$$

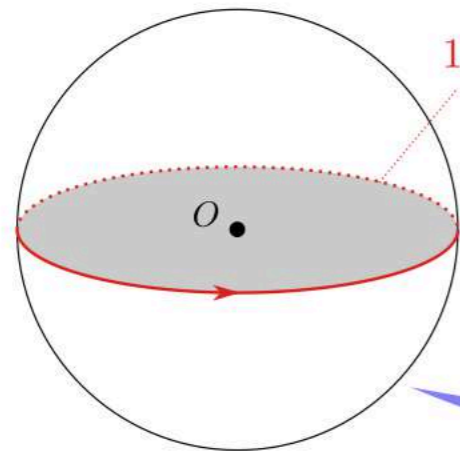
HW, S. Ono, PRB (2020)

Coupled-wire/layer argument



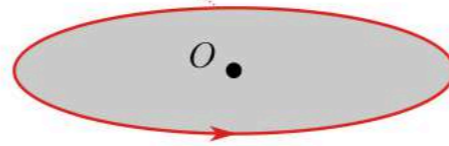
Similarity to HOTTI

(a) 3D Higher-Order TI

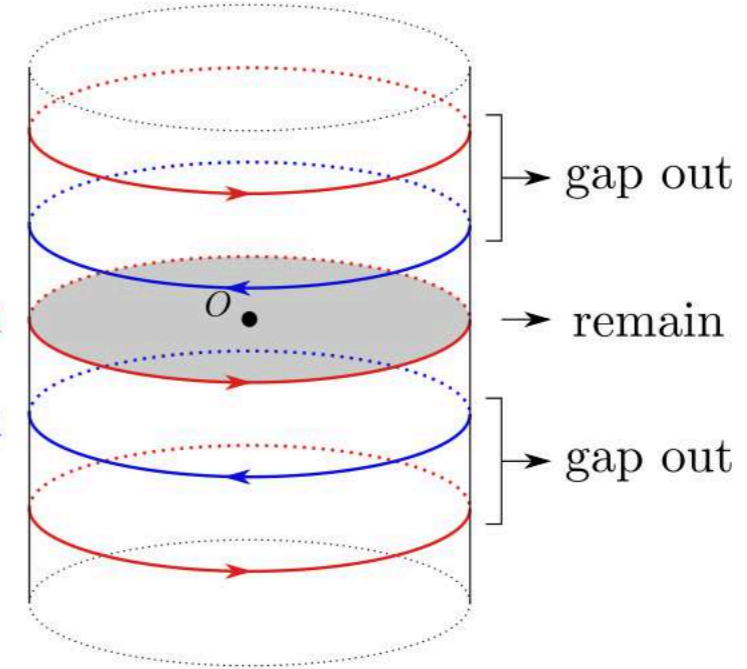


1D Chiral Edge Mode

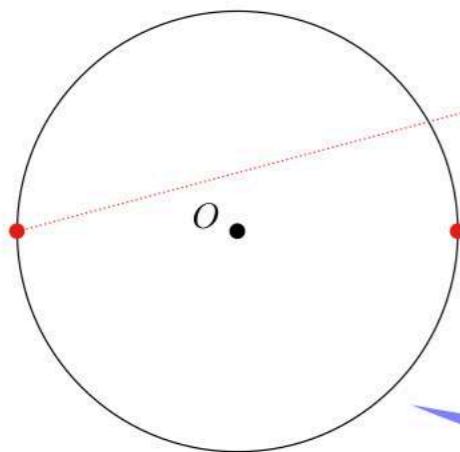
(b) 2D Chern Insulator

 $C = +1$ $C = -1$

(c)



(d) 2D Higher-Order TI

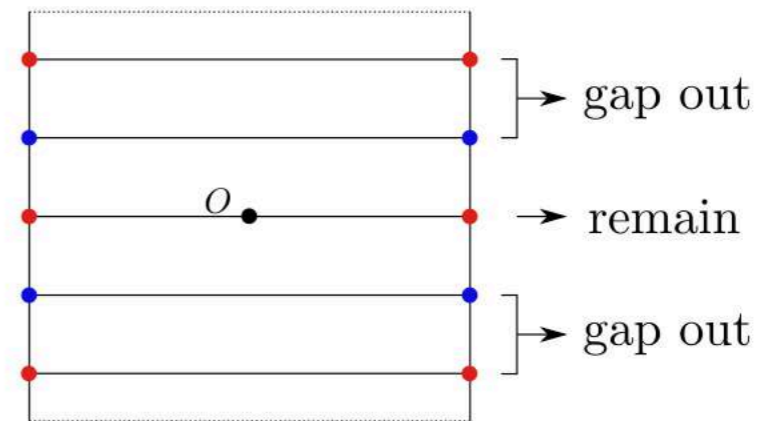


0D zero modes

(e) 1D Class AIII Insulator

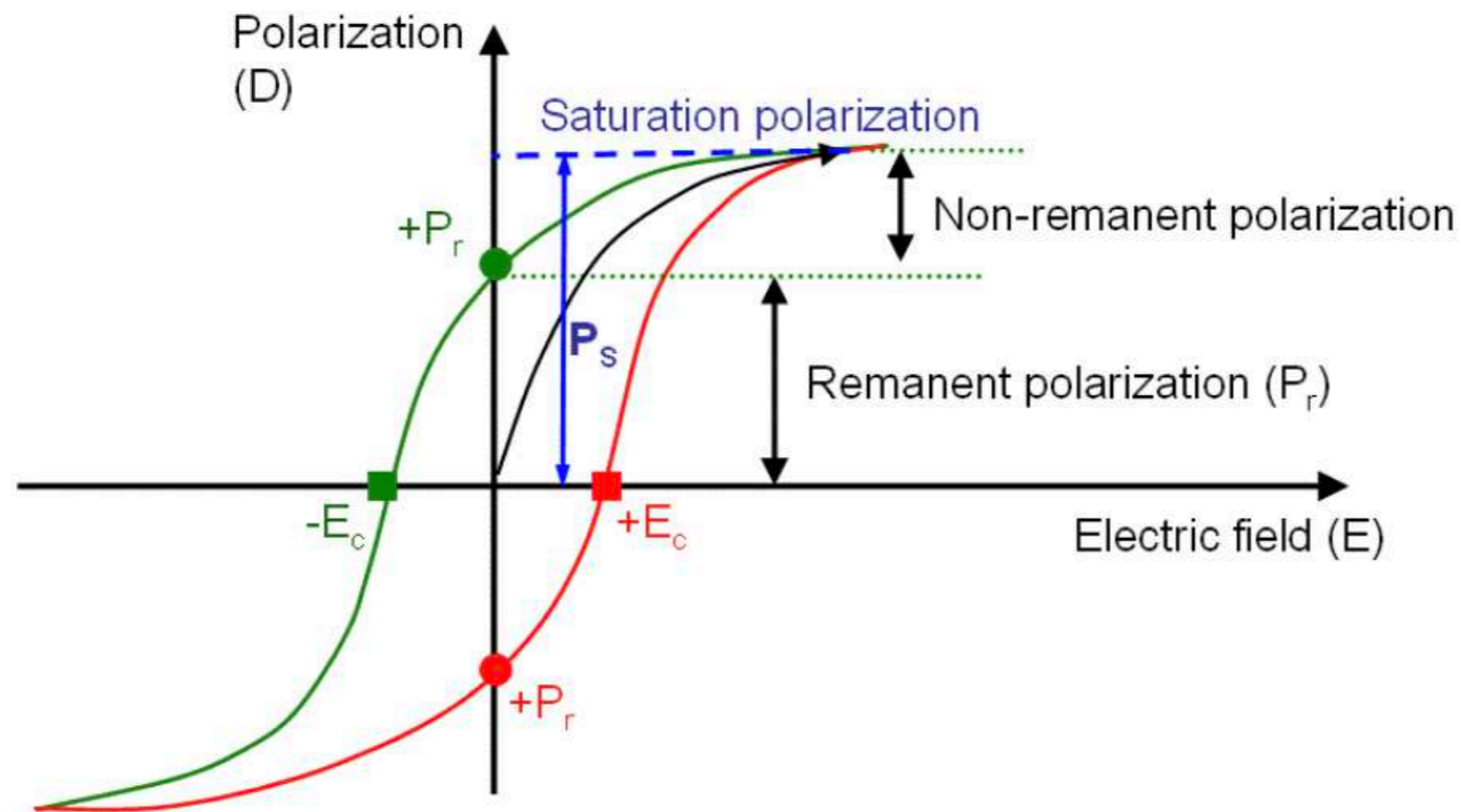


(f)



Traditional measurement of the bulk polarization

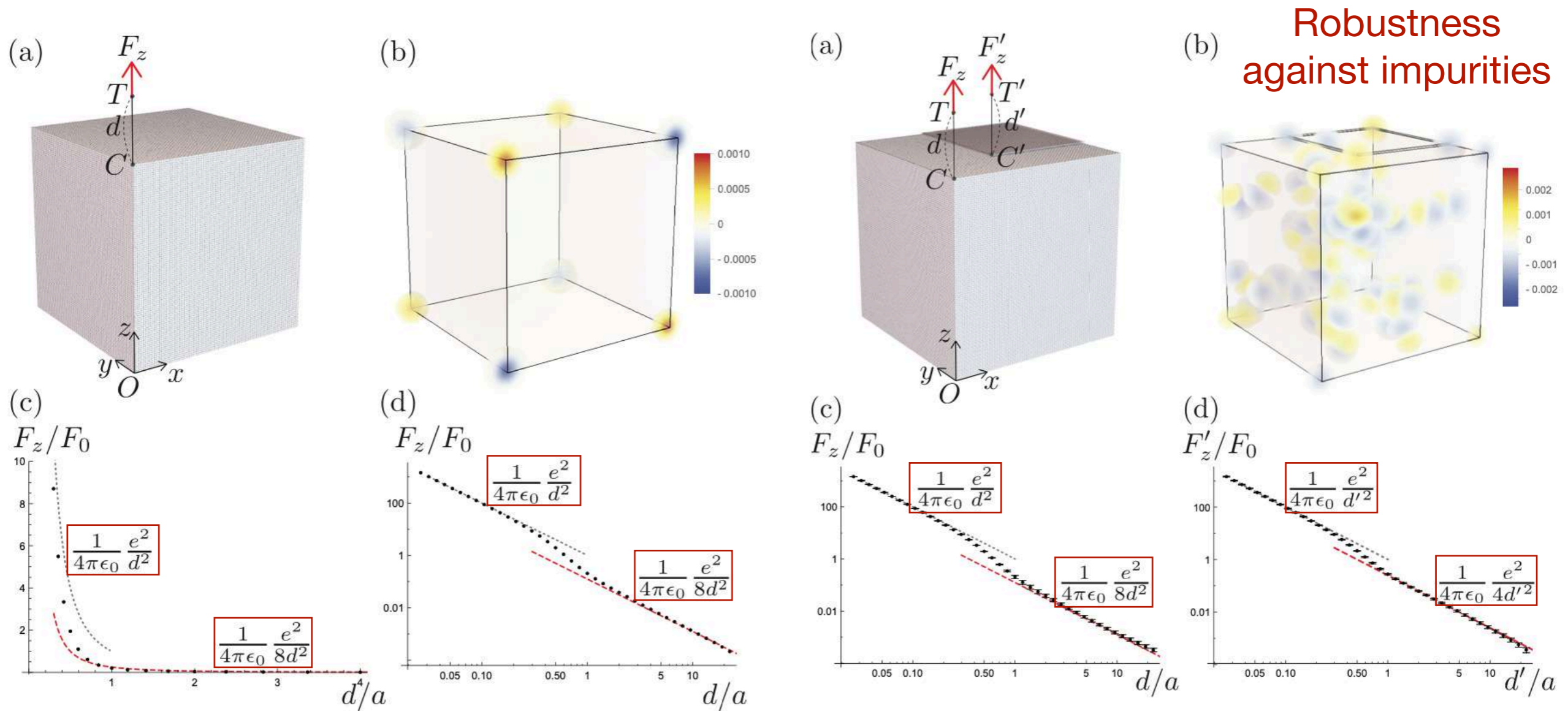
- Change a parameter and measure the electric current during the process.



$$2P_x = \int_0^T dt J_x(t)$$

Figure from <https://www.globalsino.com/EM/>

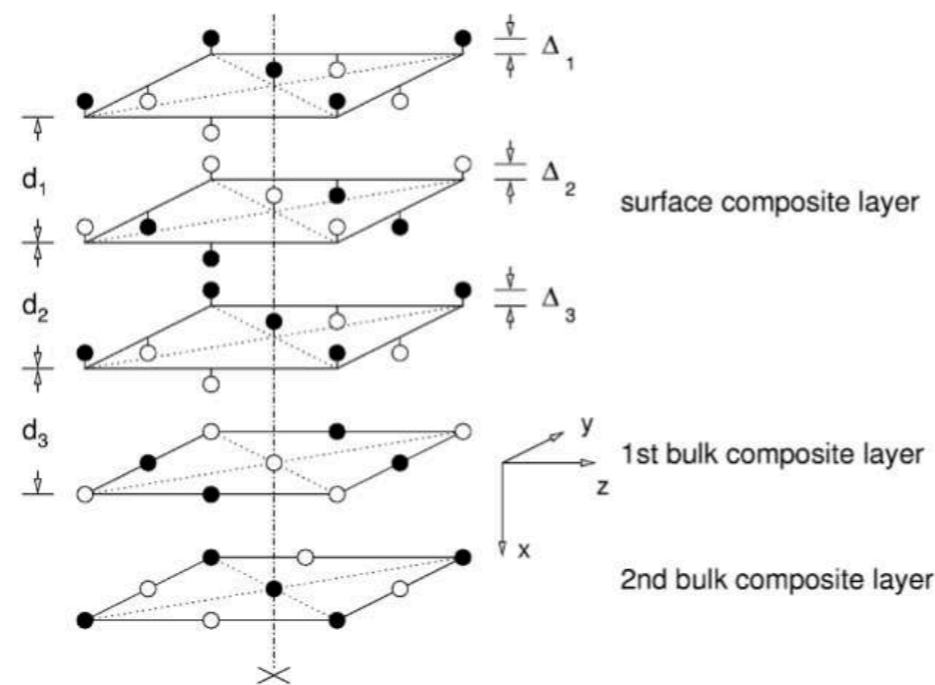
Possible direct measurement via atomic force microscope



$$F_0 \equiv \frac{e^2}{4\pi\epsilon_0 a^2} = 7.25 \times 10^{-10} \text{ kg m s}^{-2} = 725 \text{ pN} \quad \text{for } a = 5.64 \text{ \AA}$$

Corrections from surface dipoles & hinge polarizations

J. Vogt, H. Weiss / Surface Science 491 (2001) 155–168

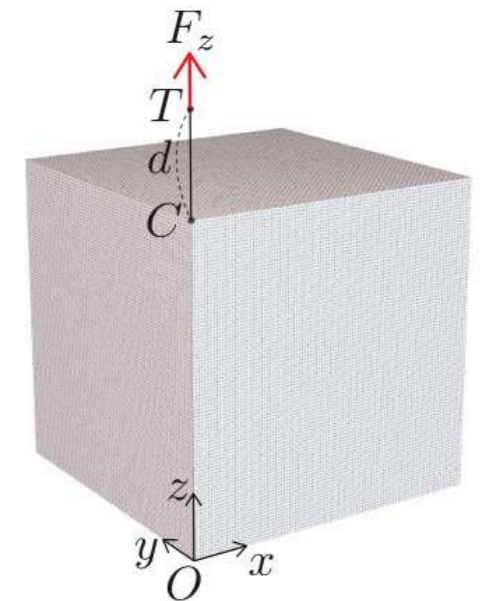


$$\mathbf{r}_0 = (0, 0, d)$$

$$\mathbf{E}(\mathbf{r}) = (0, 0, 1) \frac{Q_c}{d^2} + \left(-\frac{1}{8}, -\frac{1}{8}, \frac{1}{2}\right) \frac{4p_h + 2p_s^a + p_s^c - 2q_s}{d^2} + O(d^{-3})$$

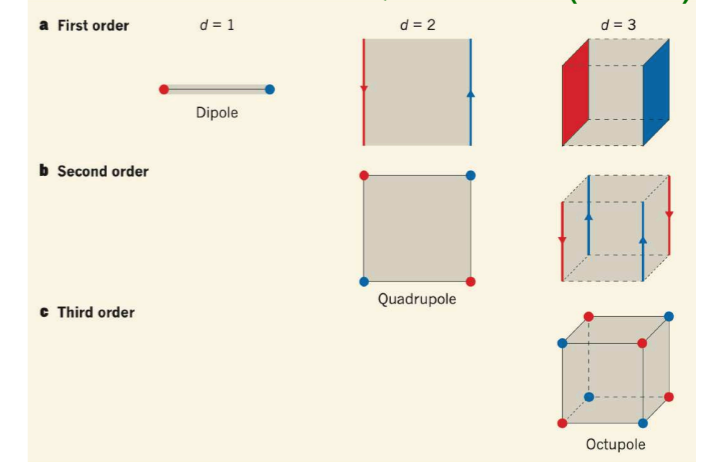
$$\mathbf{r}_0 = (d, d, d)/\sqrt{3}$$

$$\mathbf{E}(\mathbf{r}) = \frac{1}{\sqrt{3}}(1, 1, 1) \frac{Q_c}{d^2} + (1, 1, 1) \frac{3-\sqrt{3}}{4} \frac{4p_h + 2p_s^a + p_s^c - 2q_s}{d^2} + O(d^{-3})$$



Summary

M. Fruchart et al, Nature (2018)



- Topological vs Trivial

- Higher-order *topological* insulators
- Gapless *modes* on hinges / corners
- Irremovable quantum entanglement
- Higher-order *trivial* insulators
- Fractional charges on hinges / corners
- Connected to product state

- We bridged “multipole moments” and “filling anomaly”

Quadrupole moment $Q_{\text{corner}} = q_{12}^{\text{bulk}} = \int d^d r \rho_0(\mathbf{r}) \frac{xy}{a^2}$

||

Filling anomaly $Q_{\text{corner}} = \frac{1}{4}q_a = \frac{1}{4}q_b \pmod{e}$